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**Dynamické vlastnosti
spinově-polarizovaných laserů**

**Dynamical properties of
spin-polarized lasers**

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Description:

The recent highlight of spin-injected lasers for innovative applications generated an important research interest in multidisciplinary field of spintronics and photonics. In such devices the radiative recombination of spin-polarized carriers results in emission of circularly polarized photons. Control of the polarization state of emitted light is desired for a number of polarization-sensitive application. Polarization dynamics of these devices can be described using Maxwell-Bloch equations for four-level lasing systems, which include the polarization spin sublevels of the conduction and valence band. Main goals of this thesis are (i) study of the quantum transitions of spin-polarized carriers, (ii) theoretical investigation and analysis of light polarization dynamics of semiconductor spin-lasers, and (iii) application of theoretical models to novel vertical-cavity surface emitting laser structures (spin-VCSELs).

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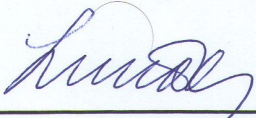
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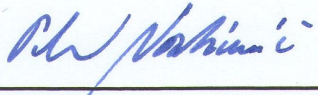
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Abstract

This bachelor thesis deals with dynamical properties of spin-polarized lasers. Because of promising high light polarization control performance, their light polarization dynamics is extensively studied. It can be done using 4-level simplified Maxwell-Bloch equations. Real spin-polarized semiconductor lasers possess complicated V(E)CSEL (Vertical-(External) Cavity Surface-Emitting Laser) geometries which additionally contain local optical anisotropies. Thus, precise modeling of dynamics is difficult and it is beyond the scope of this work to include anisotropies. Spin-laser's resonant cavities consist of Bragg reflectors, which are modeled theoretically in this thesis. Furthermore, the ellipsometric measurement of GaAs/AlAs Bragg reflector is presented. In order to solve simplified Maxwell-Bloch equations and analyze spin-laser's dynamics, one has to evaluate losses of resonant cavity, because it is an important factor defining dynamics. It was done using the connection of losses to resonator's spectral response profile which is based on Fourier analysis. Results are then discussed.

Key words: laser, spin, spin-V(E)CSEL, Bragg reflectors, Maxwell-Bloch equations, spin-lasers dynamics.

Abstrakt

Tato bakalářská práce se zabývá dynamickými vlastnostmi spinově-polarizovaných laserů. Z důvodu slibné možnosti kontroly polarizace emitovaného světla je kladen důraz na studium dynamiky polarizace emitovaného světla. Jednou z možností je řešení zjednodušených Maxwell-Blochových rovnic pro čtyř-úrovňový systém. Reálné spinově-polarizované polovodičové lasery mají komplikované V(E)CSEL (Vertical-(External) Cavity Surface-Emitting Laser) geometrie obsahující navíc optické anizotropie, což velmi komplikuje přesné modelování dynamiky. Zahrnutí anizotropií je nad rámec této práce. Rezonanční kavity spinových laserů se skládají z Braggových zrcadel, které jsou zde teoreticky modelovány. Navíc bylo provedeno elipsometrické měření Braggova zrcadla složeného z GaAs/AlAs. Abychom mohli řešit zjednodušené Maxwell-Blochovy rovnice a analyzovat tak dynamiku spinových laserů, je třeba určit ztráty rezonátoru, protože ty významně ovlivňují dynamiku. Ty bylo možné určit díky tomu, že ztráty lze určit ze spektrální odezvy rezonátoru, což vyplývá z Fourierovy analýzy. Výsledky jsou poté diskutovány.

Klíčová slova: laser, spin, spin-V(E)CSEL, Braggovo zrcadlo, Maxwell-Blochovy rovnice, dynamika spinových laserů.

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List of symbols

c	Velocity of light in vacuum
C	Lamb coupling constant
c_n	Projection of state vector onto n-th eigenvector
d_n	Thickness of n-th layer
e lh hh	Electron, light-hole and heavy-hole band carrier concentration
E_n	n-th eigenvalue of Hamiltonian operator
E_0	Electric field amplitude(scalar)
F	Number of photons
ΔG	Gain dichroism
G_n	Non-saturated gain coefficient of n-th mode
h	Planck constant
\hbar	Dirac constant
I	Intensity of light
I_n	Intensity of n-th mode
I_{sat}	Saturation intensity
L	Length of cavity
n	Number of atomic systems per unit volume or one of SFM population inversion
n_0	Refractive index of unperturbed medium
Δn	Population inversion
Δn_0	Unsaturated population inversion
Δn_{th}	Threshold population inversion
N	Number of atoms or number of layers or one of SFM population inversion
P	Pump ellipticity or probability
P_n	Electron spin polarization or probability of measuring n-th eigenstate
r_s r_p	Amplitude reflectivity coefficients for s- and p- polarization respectively
R_i	Reflective coefficient of i-th reflector
R^M R^C	Measured and calculated reflectivity coefficients respectively
$R_{i \rightarrow f}$	Probability of transition per unit of time
S	Section area
t	Time
t_{RT}	Time duration of round-trip

u_m	Amplitude of Bloch wavefunction
V	Volume
v	Velocity of light in medium of refractive index n_0
W	Pumping rate
ω	Angular frequency of light
ω_0	Atomic transition eigenfrequency
ω_R	Rabi angular frequency
\mathbf{A}	Complex amplitude
\mathbf{B}	Magnetic induction
\mathbf{D}	Electric displacement vector
\mathbf{E}	Intensity of electric field
\mathbf{E}_0	Amplitude of electric field intensity
\mathbf{H}	Magnetic field Intensity
\mathbf{H}_0	Amplitude of magnetic field intensity
\mathbf{k}	Wave vector
\mathbf{M}	Mueller matrix
\mathbf{N}	Generalized refractive index
$\tilde{\mathbf{P}}$	Complex dipole moment density
\mathbf{P}	Dipole moment density
\mathbf{P}_{at}	Dipole moment density of active atoms
\mathbf{p}	Dipole moment
\mathbf{r}	Position vector
\mathbf{S}	Poynting vector or Stokes vector
$ \psi\rangle$	State ket-vector psi
$\langle\psi $	State bra-vector psi
$ n\rangle$	n-th eigenvector
$\psi(\mathbf{r}, t)$	Wavefunction
$\uparrow \downarrow$	Spin-up and spin-down projections
$\hat{\epsilon}$	Permittivity tensor
\hat{H}	Hamiltonian operator
\hat{H}_0	Unperturbed Hamiltonian
\hat{H}_{SO}	Spin-orbit interaction Hamiltonian
$\hat{\eta}$	Electric dipole operator
$\hat{\rho}$	Density operator
\hat{P}	Projection operator
ρ_{ij}	Elements of density operator
σ_{ij}	Elements of transformed density operator
\hat{x}	Arbitrary operator
x_{mn}	Matrix element of arbitrary operator

\hat{W}	Perturbation Hamiltonian
α	Henry's coefficient
α_a	Absorption coefficient
α_e	Effective absorption coefficient
β_n	Self-saturation coefficient of n-th mode
Φ	Photon flux
Λ_n	Pumping rate of n-th level population
Λ	Pumping rate
λ	Wavelength
λ_0	Resonance wavelength
δ	Detuning
δ_{cav}	Cavity detuning
κ	Stimulated emission coupling constant
Γ	Decay rate of coherences
γ_n	decay constant of n-th level
γ_{mn}	decay constant of transition between m-th and n-th
$\tau = \frac{1}{\gamma}$	Population inversion lifetime
τ_{ph}	Photon lifetime
τ_s	Spin relaxation lifetime
τ_E	Field decay lifetime
θ_{ij}	Cross-saturation coefficients
θ	Angle of incidence
ς	Fictive conductivity
$\sigma(\nu)$	Cross section as a function of frequency
ϵ_0	Permittivity of vacuum
Ψ, Δ	Ellipsometric angles
μ	Permeability
ν	Frequency
ν_0	Resonance frequency
$\Delta\nu$	FWHM
χ	Susceptibility
$Tr \{..\}$	Trace of matrix/operator
∇	Nabla operator
\times	Vector product
$\mathbf{D}^{(n)}$	Dynamic matrix of n-th layer
$\mathbf{P}^{(n)}$	Propagation matrix of n-th layer
$\mathbf{A}^{(n)}$	Amplitude vector in n-th layer
\mathbf{e}_j	eigen-polarization of j-th mode

Chapter 1

Introduction

The nature of research in physical sciences in this century slightly differs from research conducted in the previous one. In the 20-th century humankind was able to study and understand the great variety of Nature like never before. Now, this variety manifests itself in current technologies. One of the most interesting example of such technology is laser. Laser is a device generating light using stimulated emission which is possible thanks to discrete structure of matter. The variety of laser technologies lies in the number of materials and mechanisms used to generate photons. One of the most promising photonic technologies under development are spin-polarized semiconductor lasers. The mechanism of photon generation in semiconductor lasers is based on re-combination of electrons and holes that must be described using quantum mechanics. Quantum mechanics together with special theory of relativity predicts the existence of spin which is intrinsic angular momentum of elementary particles. As well as in case of other physical quantities, angular momentum of system is conserved during certain physical processes. Such process is for example the re-combination of electron and hole after which right-circularly or left-circularly polarized photon is created. Polarization of photon is defined by projection of its angular momentum on direction of propagation. Spin-polarized lasers are interesting because we may control spin projection of injected electrons and consequently polarization of emitted light.

Despite the fact that spin-polarized lasers are under development, another class of spin-polarized devices (spin-light emitting diodes) is already used as an analytic tool in experimental spintronics[19]. One of the promise of spin-polarized lasers is that they would operate with lower threshold than their conventional counterparts [14, 19]. It was theoretically and experimentally verified [15, 16]. Next, it is for example fast modulation dynamics [17]. The experiments are being conducted using both optical and electrical pumping [7]. However, it is challenging to inject and sustain polarized electron population at room temperatures and in weak magnetic fields which is one of the reasons why the light polarization control is not as simple as it seems to be [7]. Optical anisotropies such as surface strain and interface anisotropy (T_d and C_{2V} symmetry breaking at III-IV semiconductor interface [25]) inside spin-laser structures are among other reasons [21]. The presence of anisotropies causes decay

of circular polarizations and preference for oscillation of two linear polarization modes[21, 7]. The model that describes spin-polarized laser's emission in steady-state with very high precision was developed by Fördös et al. [18]. Their modified Yeh's matrix formalism can model spin-laser emission in presence of optical anisotropies such as linear birefringence or magneto-optical anisotropy for example. However, there is a need for accurate modeling of dynamical properties of such devices.

The main goal of this thesis is to describe dynamical properties of spin-polarized lasers as it was indicated. In order to do this we have to present and discuss general laser fundamentals. Chapter 2 deals with basic ideas of laser physics and light-matter interaction. The equations that describe laser dynamics are derived using the density operator formalism. At the end of Chapter 2 we present calculations that demonstrate typical dynamical properties of lasers. Later, in Chapter 3 we describe resonant cavities used in spin-polarized lasers and ellipsometric measurement of Bragg reflector is presented. After this, we discuss quantum transitions in semiconductor structures used in spin-polarized lasers. Additionally, we calculate time-evolution of intensity of light in spin-polarized lasers using so called spin-flip model with parameters measured on real structures [7]. Finally, in Chapter 4 we present the calculation of photon lifetimes in complicated resonant cavities and we use obtained parameters during spin-polarized laser's dynamics calculations. At the end of thesis there are two appendices in which the fundamentals of non-relativistic quantum mechanics and Yeh's matrix formalism are presented. All the calculations are carried out using MATLAB.

Chapter 2

Laser Physics

2.1 LASER

2.1.1 What is a laser ?

Of all the light-sources we use, there is one with unusual and exceptional properties. It is called LASER, which stands for **L**aser **A**mplification by **S**timulated **E**mission of **R**adiation. Stimulated emission is a process in which photon interacts with excited atom, molecule or more complex system so that another photon is created. Such process must obey energy conservation law. Thus, energy of the system is reduced by the amount of energy which is equal to photon's energy. Created photon has the same energy, a polarization, a phase and a momentum as the incoming one.

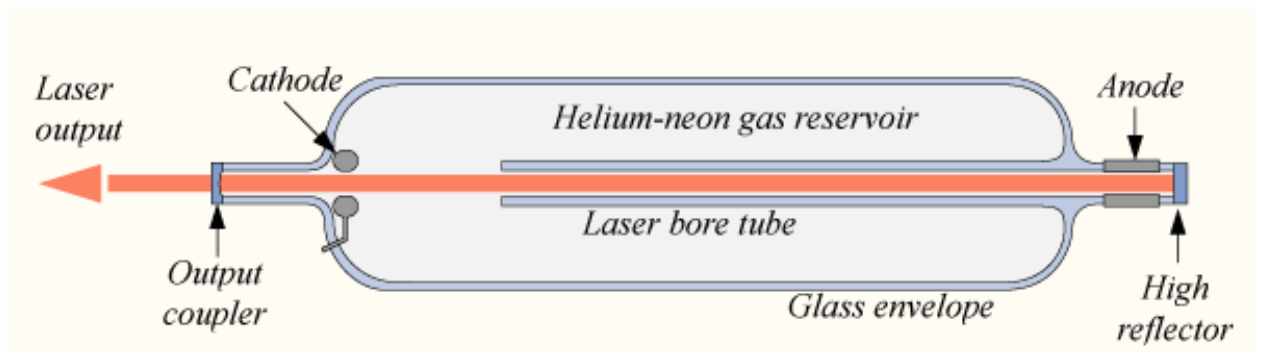


Figure 2.1: *Helium - neon laser scheme. The gain medium is formed by a mixture of helium and neon. Electrical discharges excite helium atoms which excite neon through the collisions. Laser radiation comes from transitions in neon [22].*

From a simplified technical point of view, laser consists of a gain medium, a resonant cavity and pump to power the laser (see Figure 2.1).

- Gain/active medium - It is material or a combination of materials in which specific optical transitions can be distinguished. One often wants laser to be working at certain wavelength and this can be approximately done by choosing the right gain medium.

There are solid, liquid, gas active media. In the semiconductor lasers it can be system of quantum wells or even quantum dots. When we are talking about active media it should be noted that so called **population inversion** must be established to make it amplifying. It is state when the number of excited atomic systems in gain medium is larger than the number of systems in the ground state. To be precise in lasers the lower energy level does not have to be the ground state. Sometimes the quantity called population inversion is used and it denotes to difference of such populations [6].

- Pump - This basic element of lasers is required for achieving the population inversion. We can pump lasers using thermal energy, optical or for example through electrical current.
- Resonant cavity - The role of resonant cavity is to keep photons inside laser for the longest possible time interval. There are for example atoms of active medium in the cavity and photons going back and forth. If there was no resonator or resonator with very low reflectivity, stimulated emission would end very quickly because photons would escape cavity. The chose of resonator is very important as well because from classical electromagnetic point of view there are discrete values of wavelengths that can exist in resonators.

Thanks to the process of stimulated emission in a gain medium and resonator feedback lasers emit radiation of a very high degree of coherence and its spectra have a very small linewidth. Let us consider that we have a light source and we are studying light which is emitted by it. If the phase and the frequency of incoming light is chaotically changing we can say that the source produces incoherent light. The more predictable is phase and frequency the higher is the degree of coherence of light. There is a temporal and a spatial coherence. The only difference is that we study the light in a time or in a space respectively. They are widely used as scientific instruments for example in laser spectroscopy because of its small linewidth. There is for example a possibility to study very small energy differences in molecules using laser. The coherence of laser radiation is used in interferometric applications. Another laser applications are in optical communications, information technologies or medicine and many more [2].

Finally, if we wanted to answer the question *What is a laser ?*, we would say *It is device which uses stimulated emission to generate nearly monochromatic collimated light of very high degree of coherence* [8].

2.1.2 History

Development of scientific knowledge is not that straightforward as we often imagine. This was the case of laser as well. There were lot of physicists that made significant contributions to laser physics but we want to mention just the most important ones.

Despite the fact that Albert Einstein was not satisfied with quantum - mechanical description of physical reality, he helped to develop it. Besides his other famous works on old quantum theory, in the year 1917 he published paper named "The quantum theory of radiation" [5] in which he introduced stimulated emission and absorption. In this paper he investigated exchange of energy between atoms and photon field in the thermal equilibrium. Performing this analysis he was not only able to re - derive famous Planck's radiation law, but introduced A and B coefficients which help to calculate probability densities of optical transitions and in fact established theoretical foundations of laser.

For a certain amount of time the developments in the field of coherent electromagnetic waves amplification was going slowly. Meanwhile, the principle of stimulated emission was experimentally proved. After that, in the 1950s Charles Townes, Nikolay Basov and Aleksandr Prokhorov developed devices which were able to coherently (but not continuously yet) amplify microwave radiation. It was called **maser**. Not long after the discovery of the first maser Charles Townes and Arthur Schawlow formulated conditions in which continuous amplification of light would be possible. Finally, in the year 1960 Theodore Maiman constructed the first working laser. It was a solid-state laser with ruby crystal as an active medium and the laser was pumped optically by a flash lamp [2].

2.1.3 Mathematical description

It is well - known in theoretical physics that single phenomena can be described in many ways, using numerous frameworks or models. Model is thought to be successful if it gives predictions which agree with correctly performed experiment. When it comes to laser physics, there are at least four approaches which agree with experiments and we may use them to describe basic interactions in laser. We should mention that it is not sharp classification and following approaches can be combined with each other. Now, we are going to discuss them shortly [8, 1].

- **Classical oscillator model** - The first approach in laser physics is fully classical and is better known as the Lorentz model. Originally it was developed to calculate permittivity or refractive index of dielectric materials. The main idea is that electrons in gain medium are connected to nuclei with idealized springs that have resonant frequency of given atomic transition. If such system interacts with plane electromagnetic wave, electron on a spring is driven by harmonic electric field. It can be derived that field induces existence of electric dipoles and material polarization respectively so that waves going through medium are amplified if there exists population inversion. The model is easy to work with because we need only elementary differential and integral calculus. However, there are disadvantages too which arise from the fact that it is purely classical. Many parameters should be achieved experimentally or using not so simple quantum-mechanical calculations [8].

- **Old quantum theory** - The previous model of basic interactions in lasers works with physical quantities such as electric field intensity, polarization density and population inversion. Here, the situation is a little bit different. The interactions in laser active medium are described using the number of photons and population inversion. The approach is based mainly on Einstein's work on quantum theory of radiation, where he was able to postulate probability expressions for different kind of transitions when atoms are illuminated by light of given spectral energy density. Again, the model contains quantities that cannot be achieved by the model alone. The main advantage is that it is very easy to construct so called **rate equations**, which describe laser dynamics in the simplest possible manner. Here, the rate equations are coupled differential equations which couple together the number of photons in cavity (or number of photons per volume unit) with population inversion.
- **Semi-classical model** - As one can expect we want to discuss the approach in which some aspects are quantum and other are classical. More precisely, atoms of gain medium are being treated quantum-mechanically but electromagnetic field is classical. It is model we are using in this thesis and it works with **the density matrix/operator** which we are going to define and describe in the next section. Of course, the approach is more general than the previous ones and reflects much better on what is going on in lasers. Physical quantities that are being described are the same as in the classical model.
- **Fully-quantum treatise** - Here, even electromagnetic field must be quantized so the quantum electrodynamics must be incorporated. It is the most complete and rigorous description of light - matter interaction. In fact, all the aspects of laser physics can be calculated using quantum electrodynamics ab-initio which could be in practice very difficult [2].

2.2 Dynamics of open quantum system

2.2.1 A single quantum system in electromagnetic field

Let us have two-level system. For example some idealized atom or molecule with only two non-degenerated eigenstates for simplicity. First, we assume that system is isolated. If such system did not interact with environment, the time-evolution of system would be completely known from the solution of the time-dependent Schrödinger equation. We would obtain[12]

$$|\psi(t)\rangle = c_1 \cdot |1\rangle \exp(-i\frac{E_1}{\hbar}t) + c_2 \cdot |2\rangle \exp(-i\frac{E_2}{\hbar}t), \quad (2.1)$$

where $|\psi(t)\rangle$ is the state vector of system, c_1 , c_2 are projections of state vector on eigenstates $|1\rangle$ and $|2\rangle$ of system. E_1 and E_2 are energies of eigenstates. It is important to note that

$\frac{E_2 - E_1}{\hbar}$ is equal to angular frequency ω_0 of photon which is created when transition from state $|2\rangle$ to state $|1\rangle$ occurs. Next, because we want to understand basic light - matter interaction, imagine that our two - level system is illuminated by a monochromatic light which may be represented as plane electromagnetic wave of angular frequency ω that is close to ω_0 . We treat light as a classical electromagnetic wave but atomic system quantum mechanically. In the massive framework of quantum mechanics we can find so called perturbation theory which is able to deal with situations like our. The electromagnetic wave can be understood as a perturbation of atomic system which is somehow influenced by it and we will see how.

We should construct interaction Hamiltonian. In this case it is very simple, we introduce electric dipole operator $\hat{\eta}$. Interaction Hamiltonian is [6]

$$\hat{W}(t) = -\hat{\eta} \cdot \mathbf{E}(t) = -\hat{\eta} \cdot (\mathbf{A}^* e^{i\omega t} + \mathbf{A} e^{-i\omega t}). \quad (2.2)$$

\mathbf{E} is the intensity of electric field and \mathbf{A} is the complex amplitude of electromagnetic wave. \mathbf{A}^* is the complex conjugate of \mathbf{A} . There must be added complex conjugate because every operator in quantum mechanics must be Hermitian to be observable. Now we can write down modified Schrödinger equation

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = [\hat{H}_0 + \hat{W}(t)] |\psi(t)\rangle, \quad (2.3)$$

where \hat{H}_0 is Hamiltonian of unperturbed system. It can be assumed that generally

$$|\psi(t)\rangle = \sum_n c_n(t) |n(t)\rangle. \quad (2.4)$$

We can insert this general solution into quantum-mechanical equation of motion, evaluate derivatives and cancel the same terms on both sides of equation. Then we multiply both sides by m -th eigenvector and perform summation so we have

$$i\hbar \dot{c}_m(t) = \sum_n c_n(t) \cdot W_{mn}(t) \cdot e^{-i\omega_0 t}. \quad (2.5)$$

Detailed derivation is presented in Appendix A. $W_{mn}(t)$ is a matrix element of $\hat{W}(t)$. The great advantage is that we are working with only two - dimensional Hilbert space and it is clear that obtained equation is in fact set of differential equations which we can write down [6]

$$\dot{c}_1 = \frac{i}{2} c_2 (\omega_R^* e^{i\omega t} + \omega_R e^{-i\omega t}) e^{-i\omega_0 t}, \quad (2.6)$$

$$\dot{c}_2 = \frac{i}{2} c_1 (\omega_R^* e^{i\omega t} + \omega_R e^{-i\omega t}) e^{i\omega_0 t}. \quad (2.7)$$

Now we should mention two things. We could obtain this set of equations by making coefficients c_i in (2.1) time-dependent and inserting general solution to Schrödinger equation. It is often valuable to find not just one derivation. The second interesting aspect of this set

of equation is that when we set $\omega = \omega_0$ our system will be oscillating between two eigenstates with frequency [12]

$$\omega_R = \frac{2\eta\mathbf{A}}{\hbar}, \quad (2.8)$$

where ω_R is **Rabi angular frequency**. In the language of the quantum mechanics it means that probability of measurement of each state is time-dependent and may be described by a harmonic function in this case. At the certain moment it is more probable that the system is in a state $|1\rangle$ but later the orthogonal eigenstate can be more probable and so on. So the system is driven by field, oscillating between its eigenstates and every time it makes transition from $|2\rangle$ to $|1\rangle$ photon is created. Generally $\omega \neq \omega_0$ but analysis of this case is not difficult and one has to be familiar only with classical harmonic oscillators. For more details, see Appendix A.

It is obvious that the laser's gain medium does not consist of just one atomic system. It is even more obvious that we do not know in what states they are so we have to use some statistical approach. In the year 1927 John von Neumann, independently with soviet physicist Lev Landau, developed density operator formalism which is in fact more general description of reality when it comes to many particles. Now we have to go beyond the Schrödinger equation and discuss density operator formalism [4, 6].

2.2.2 The density operator

As it was indicated, if we are studying a single atomic system we can use the Schrödinger equation. However, it is not useful approach if there are billions and billions of systems. It would be a coincidence if they were all "in phase" from a quantum-mechanical point of view. Thus, generally there is dispersion and we have to incorporate formalism which combines elements of quantum and statistical physics [12]. Let us first define the density operator, mention some properties and then we will discuss its meaning for laser physics. Mathematical definition of density operator is

$$\hat{\rho}(t) = |\psi(t)\rangle \langle\psi(t)|. \quad (2.9)$$

It can be proved that density operator may be represented by a matrix with matrix elements in the $\{|n\rangle\}$ basis [12]:

$$\rho_{mn}(t) = \langle m | \hat{\rho}(t) | n \rangle = \langle m | \psi(t) \rangle \langle \psi(t) | n \rangle = c_m(t) c_n^*(t). \quad (2.10)$$

The meaning of each matrix element will be discussed later.

Now, we want to show how to obtain mean value of some operator in the density matrix formalism. In order to do this, let us recall what is general principle of calculating operator's mean value on the example of an arbitrary operator \hat{x} :

$$\langle \hat{x} \rangle (t) = \langle \psi(t) | \hat{x} | \psi(t) \rangle = \sum_m \sum_n c_m^*(t) c_n(t) \langle m | \hat{x} | n \rangle = \sum_m \sum_n c_m^*(t) c_n(t) x_{mn}. \quad (2.11)$$

Note, that the result can be re - written as

$$\langle \hat{x} \rangle (t) = \sum_{m,n} \langle \psi(t) | m \rangle \langle n | \psi(t) \rangle \langle m | \hat{x} | n \rangle = \sum_{m,n} \langle n | \psi(t) \rangle \langle \psi(t) | m \rangle \langle m | \hat{x} | n \rangle. \quad (2.12)$$

Recalling, that $\sum_m |m\rangle \langle m|$ is the projection operator which can be always taken out of the equation and additionally that $|\psi(t)\rangle \langle \psi(t)|$ is the density operator, we can write

$$\langle \hat{x} \rangle (t) = \sum_n \langle n | \hat{\rho}(t) \hat{x} | n \rangle. \quad (2.13)$$

The interpretation is very easy, it equals to the trace of the matrix because it a sum of diagonal elements. Finally, we found out that mean value of an arbitrary operator in the density matrix formalism is equal to [12]

$$\langle \hat{x} \rangle (t) = Tr \{ \hat{\rho}(t) \hat{x} \}. \quad (2.14)$$

We want to mention that the need for Hermitian operators in quantum mechanics has interesting consequence. If we take a look at non-diagonal matrix elements equation $\rho_{mn} = \rho_{nm}^*$ must be fulfilled.

One can ask that *if the density matrix is generally time - dependent, how we will calculate its time - evolution?*. Let us first evaluate a derivative of the density operator

$$\frac{d}{dt} \hat{\rho}(t) = \frac{d}{dt} (|\psi(t)\rangle \langle \psi(t)|) = \left(\frac{d|\psi(t)\rangle}{dt} \right) \langle \psi(t)| + |\psi(t)\rangle \left(\frac{d\langle \psi(t)|}{dt} \right). \quad (2.15)$$

Next, we should take the Schrödinger equation and its Hermitian conjugate form

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H} |\psi(t)\rangle, \quad \Rightarrow \quad -i\hbar \frac{d\langle \psi(t)|}{dt} = \langle \psi(t)| \hat{H}. \quad (2.16)$$

If we insert the derivatives of bra and ket vectors into equation (2.15) we obtain

$$\frac{d}{dt} \hat{\rho}(t) = \frac{1}{i\hbar} \left[\hat{H} |\psi(t)\rangle \langle \psi(t)| - |\psi(t)\rangle \langle \psi(t)| \hat{H} \right] = \frac{1}{i\hbar} \left[\hat{H} \hat{\rho}(t) - \hat{\rho}(t) \hat{H} \right]. \quad (2.17)$$

The term $\hat{H} \hat{\rho}(t) - \hat{\rho}(t) \hat{H}$ is commutator which can be written in a compact form as $[\hat{H}, \hat{\rho}(t)]$. We obtained one of the most important equation of this thesis. It is called **von Neumann equation** or sometimes Liouville equation [12]:

$$i\hbar \frac{d}{dt} \hat{\rho} = [\hat{H}, \hat{\rho}]. \quad (2.18)$$

Let us discuss on a few lines the meaning of diagonal and off-diagonal elements in density matrix. If we take a look on diagonal ones it will be seen at the first sight that $\rho_{nn}(t) = c_n(t)c_n^*(t) = |c_n(t)|^2$, which is probability of finding system in n-th eigenstate. If there are for example N atomic systems in active medium of laser, $N\rho_{nn}(t)$ denotes to the number of systems in n-th eigenstate. For this reason diagonal elements are called **populations**.

When it comes to non-diagonal elements the situation is more difficult. However, we are familiar with terms like $c_m(t)c_n^*(t)$. Those are interference cross terms and $\rho_{mn}(t)$ is average of interference terms between m-th and n-th eigenstates. It is good to use analogy from optics where there is required certain degree of coherence of optical field so interference effects may be distinguished. Non-diagonal elements of density matrix are called **coherences**. When $\rho_{mn}(t) \neq 0$ there are some interference effects between m-th and n-th eigenstates [12]. In the case of laser physics (or more precisely the gain medium), one can imagine such situation like there are constantly going on transitions between eigenstates and thus, atomic systems are interacting with electromagnetic field in cavity, influencing field and vice versa. In the following sections we are going to use density operator formalism to derive set of equations describing laser dynamics [6].

2.2.3 Bloch equations

At this point we want to go back to two - level systems and apply the density matrix formalism to our original problem which was treated using Schrödinger equation and time - dependent perturbation theory. Outline of the problem is to describe dynamics of two-level atomic systems in laser gain medium if it is illuminated by a monochromatic plane wave. We want to note that it may seem paradoxical because as we will see later-optically pumped laser consisting of two-level active medium cannot work. All we need is to write-down the density matrix for two-level system and complete Hamiltonian. So, the density matrix is

$$\hat{\rho}(t) = \begin{pmatrix} \rho_{11}(t) & \rho_{12}(t) \\ \rho_{21}(t) & \rho_{22}(t) \end{pmatrix}. \quad (2.19)$$

From the linearity of quantum-mechanical operators it can be deduced that complete Hamiltonian will be sum of isolated system's Hamiltonian and interaction Hamiltonian. Diagonalized Hamiltonian of isolated system is

$$\hat{H}_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}. \quad (2.20)$$

In order to construct the interaction Hamiltonian, we just should recall that in fact we worked with it already. However, it would be good to discuss for a while some of its properties. It can be written as

$$\hat{W}(t) = - \begin{pmatrix} \eta_{11} & \eta_{12} \\ \eta_{21} & \eta_{22} \end{pmatrix} \mathbf{E}(t). \quad (2.21)$$

Due to the parity of eigenvectors in the electric dipole operator's matrix elements the only non-zero elements are non-diagonal. Eigenvectors must have opposite parity in order to make given matrix element non-zero [12]. For example $\langle 1 | \hat{\eta} | 1 \rangle$ must be equal to zero. It can be checked directly taking for example wavefunctions of hydrogen atom and calculating

matrix elements of electric dipole operator, which would be in fact evaluation of integrals. Finally, the interaction Hamiltonian takes the following form

$$\hat{W}(t) = \begin{pmatrix} 0 & -\eta \mathbf{E}(t) \\ -\eta \mathbf{E}(t) & 0 \end{pmatrix}. \quad (2.22)$$

where we supposed that $\eta = \eta_{12} = \eta_{21}$. It means that η is real and hermicity of operator is accomplished. The complete Hamiltonian is

$$\hat{H}(t) = \hat{H}_0 + \hat{W}(t) = \begin{pmatrix} E_1 & -\eta \mathbf{E}(t) \\ -\eta \mathbf{E}(t) & E_2 \end{pmatrix}. \quad (2.23)$$

At this moment, we have all we need to start working with von Neumann equation. Let's begin with inserting Eqs. (2.19) – (2.23) into Eq. (2.18)

$$i\hbar \frac{d}{dt} \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \left[\begin{pmatrix} E_1 & -\eta \mathbf{E}(t) \\ -\eta \mathbf{E}(t) & E_2 \end{pmatrix}, \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \right]. \quad (2.24)$$

Simply evaluating commutator: multiplying matrices, we get the following set of differential equations

$$i\hbar \frac{d}{dt} \rho_{11} = \eta(\mathbf{A}^* e^{i\omega t} + \mathbf{A} e^{-i\omega t})(\rho_{12} - \rho_{21}), \quad (2.25)$$

$$i\hbar \frac{d}{dt} \rho_{22} = \eta(\mathbf{A}^* e^{i\omega t} + \mathbf{A} e^{-i\omega t})(\rho_{21} - \rho_{12}), \quad (2.26)$$

$$i\hbar \frac{d}{dt} \rho_{12} = (E_1 - E_2)\rho_{12} + \eta(\mathbf{A}^* e^{i\omega t} + \mathbf{A} e^{-i\omega t})(\rho_{11} - \rho_{22}), \quad (2.27)$$

$$i\hbar \frac{d}{dt} \rho_{21} = (E_2 - E_1)\rho_{21} + \eta(\mathbf{A}^* e^{i\omega t} + \mathbf{A} e^{-i\omega t})(\rho_{22} - \rho_{11}). \quad (2.28)$$

This set of equations has a certain properties we want to discuss. First, we see that the last two of the equations are conjugate to each other as we should be expected from hermicity of quantum-mechanical operators. Next, we see that $\dot{\rho}_{11} = -\dot{\rho}_{22}$, it can be easily shown using following calculation:

$$\rho_{11} + \rho_{22} = 1. \quad (2.29)$$

Now, we simply evaluate derivative of entire equation

$$\frac{d}{dt} \rho_{11} + \frac{d}{dt} \rho_{22} = 0 \quad \Rightarrow \quad \frac{d}{dt} \rho_{11} = -\frac{d}{dt} \rho_{22}. \quad (2.30)$$

Because of these two properties of our set of equations we continue the derivation only with $\dot{\rho}_{11}$ and $\dot{\rho}_{21}$. Since we know that $\hbar\omega_0 = E_2 - E_1$ and $\hbar\omega_R = 2\eta\mathbf{A}$ equations may be transformed into

$$\frac{d}{dt} \rho_{11} = \frac{i}{2}(\omega_R^* e^{i\omega t} + \omega_R e^{-i\omega t})(\rho_{21} - \rho_{21}^*), \quad (2.31)$$

$$\frac{d}{dt} \rho_{21} = -i\omega_0 \rho_{21} - \frac{i}{2}(\omega_R^* e^{i\omega t} + \omega_R e^{-i\omega t})(\rho_{22} - \rho_{11}). \quad (2.32)$$

It is the right time to discuss very special approximation we are going to make which is called **the rotating-wave approximation** [12, 6]. It is clear that the light-matter interaction we

are studying has the resonance frequency. It was shown earlier when we were working with Schrödinger equation. The light interacting with system should have frequency near the resonance point to influence it. So if we time-average all terms in equations we will find out that quickly-oscillating terms (compared to terms oscillating at nearly resonance frequency) have nearly no effect on atomic system. Such averaging can be performed using the following transformation [6]:

$$\sigma_{21} = \rho_{21} e^{i\omega t}. \quad (2.33)$$

We would say that in the complex plane we transformed our reference frame to the frame rotating with wave. This approximation is well-known in the atomic physics and experimentally verified. Thus, equations become

$$\frac{d}{dt}\rho_{11} = \frac{i}{2}(\omega_R^* \sigma_{21} - \omega_R^* \sigma_{21}^* e^{i2\omega t} + \omega_R \sigma_{21} e^{-i2\omega t} - \omega_R \sigma_{21}^*), \quad (2.34)$$

$$\left(\frac{d\sigma_{21}}{dt} - i\omega\sigma_{21}\right) e^{-i\omega t} = -i\omega_0\sigma_{21}e^{-i\omega t} - \frac{i}{2}(\omega_R^* e^{i\omega t} + \omega_R e^{-i\omega t})(\rho_{22} - \rho_{11}). \quad (2.35)$$

Now, we just cancel fast-oscillating terms and we introduce $\delta = \omega - \omega_0$ which is so called detuning frequency and is equal zero at resonance. After doing so, we have

$$\frac{d}{dt}\rho_{11} = \frac{i}{2}(\omega_R^* \sigma_{21} - \omega_R \sigma_{21}^*), \quad (2.36)$$

$$\frac{d}{dt}\sigma_{21} = i\delta\sigma_{21} - \frac{i}{2}\omega_R(\rho_{22} - \rho_{11}). \quad (2.37)$$

As far as we know, there are two problems with achieved equations. The first is that they describe some quantities that are difficult to imagine. This complication will be corrected in the next section. The second problem is that they are able to describe real situations only partially. In the real atomic systems there are constantly going on relaxation mechanisms, which arises for example from collisions of atoms. We should recall that in the beginning, when we were talking about parts of lasers, we mentioned a pump. In the laser systems energy levels are being "supplied" with electrons. If we are talking about parts of lasers, one of the most important part is resonator cavity which has of course major influence on the lasing process. All those phenomena must be included in our equations and we will do it phenomenologically by introducing parameters described below ($\Lambda_1, \Lambda_2, \gamma_1, \gamma_{21}, \gamma_2, \Gamma$). Finally, our equations become [6]

$$\frac{d}{dt}\rho_{11} = \Lambda_1 - \gamma_1\rho_{11} + \gamma_{21}\rho_{22} + \frac{i}{2}(\omega_R^* \sigma_{21} - \omega_R \sigma_{21}^*), \quad (2.38)$$

$$\frac{d}{dt}\rho_{22} = \Lambda_2 - \gamma_2\rho_{22} - \frac{i}{2}(\omega_R^* \sigma_{21} - \omega_R \sigma_{21}^*), \quad (2.39)$$

$$\frac{d}{dt}\sigma_{21} = -\Gamma\sigma_{21} + i\delta\sigma_{21} - \frac{i}{2}\omega_R(\rho_{22} - \rho_{11}). \quad (2.40)$$

Those are very famous **Bloch equations**. Originally, Felix Bloch introduced them phenomenologically to describe nuclear magnetization as a function of time. He was studying

nuclear magnetic resonance then, not lasers. However, they are formally basically the same so this is the reason they are called Bloch equations.

Let us now make a comment on the meaning of each term in Bloch equations. As we will see it is very fruitful and important to be familiar with this type of equations, especially when one is working with the rate equations.

- Λ_1, Λ_2 - those are the pumping rates. Speaking in the language of quantum mechanics, they tell us how many atomic systems are converted into states $|1\rangle$ and $|2\rangle$ respectively per unit of time using external mechanisms. In practice, it could be normalized electric current or number of electrons excited into given energetic levels per second by some source of thermal energy. Very often upper levels are pumped by another source of light, sometimes even lasers.
- γ_1 - it is coefficient of relaxation or decay of $|1\rangle$ state's population. The single coefficient may represent numerous mechanisms of relaxation caused by collisions or spontaneous emission [1]. Usually it is obtained experimentally because laser media consist sometimes of very complex atomic or molecular systems. Let us assume that term $-\gamma_1\rho_{11}$ would be the only term of (2.38):

$$\frac{d\rho_{11}}{dt} = -\gamma_1\rho_{11} \Rightarrow \rho_{11}(t) = \rho_{11}(0)e^{-\gamma_1 t}.$$

As we see, its solution would be exponential decay as for example in case of radioactivity. Of course the coefficient is meaningful only if $|1\rangle$ is not a ground state.

- γ_2, γ_{21} - the meaning of those coefficients is the same as in case of γ_1 but there is one interesting aspect of them. γ_2 denotes to overall decay rate coefficient of ρ_{22} . However, we saw that decay coefficients represent many different mechanisms phenomenologically. Then, γ_2 can be written as a sum of many coefficients

$$\gamma_2 = \sum_i \gamma_{2i}.$$

One of those coefficients is γ_{21} which represents decay when $|2\rangle$ transits to $|1\rangle$.

- Γ - finally, this coefficient is associated with decay of coherences which are hard to imagine but in the next section we will give them exact physical interpretation.

2.3 Maxwell-Bloch equations

In the previous section we dealt with light-matter interaction. We presented derivation of the Bloch equations but they lack clear physical interpretation of some quantities. To do this, one has to combine quantum - mechanical nature of matter with Maxwell equations. Now we will see, how exactly optical field inside resonant cavity influences active medium and how waves are amplified from electrodynamic point of view.

2.3.1 Macroscopic polarization

Let us recall that even purely classical theory of light amplification predicts that electromagnetic waves induce macroscopic polarization of active medium. We know that macroscopic polarization is defined as

$$\mathbf{P}_{at} = \frac{d\mathbf{p}}{dV}, \quad (2.41)$$

where \mathbf{p} is a dipole moment and dV is a volume element. The index 'at' comes from the fact that it is part of macroscopic polarization that comes only from active atoms that are responsible for lasing process. The equation for polarization may be rewritten

$$\frac{d\mathbf{p}}{dV} = \frac{d}{dV}(N \langle \mathbf{p} \rangle) = \frac{dN}{dV} \langle \mathbf{p} \rangle = n \langle \mathbf{p} \rangle, \quad (2.42)$$

Atomic macroscopic polarization is equal to atomic density(n) times mean value of electric dipole moment($\langle \mathbf{p} \rangle$). Here the correspondence between quantum and classical physics can be seen. According to Eq. (2.14) from the density operator formalism, the calculation continues as

$$n \langle \mathbf{p} \rangle = n Tr \{ \hat{\rho} \hat{\eta} \}, \quad (2.43)$$

where $\hat{\rho} \hat{\eta}$ is operator:

$$\hat{\rho} \hat{\eta} = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \begin{pmatrix} 0 & \eta \\ \eta & 0 \end{pmatrix} = \begin{pmatrix} \rho_{12}\eta & \rho_{11}\eta \\ \rho_{22}\eta & \rho_{21}\eta \end{pmatrix} \Rightarrow n Tr \{ \hat{\rho} \hat{\eta} \} = n\eta(\rho_{21}^* + \rho_{21}). \quad (2.44)$$

We know that complex number $\rho_{21}^* + \rho_{21}$ is equal to $2Re(\rho_{21})$. Remembering that $\rho_{21} = \sigma_{21}e^{-i\omega t}$ we obtain macroscopic polarization that comes from active atoms:

$$\mathbf{P}_{at} = 2n\eta Re(\sigma_{21}e^{-i\omega t}). \quad (2.45)$$

Similarly as in case of electric field intensity, we can write that

$$\mathbf{P}_{at}(t) = \tilde{\mathbf{P}}^*(t)e^{i\omega t} + \tilde{\mathbf{P}}(t)e^{-i\omega t} = 2Re(\tilde{\mathbf{P}}e^{-i\omega t}), \quad (2.46)$$

where $\tilde{\mathbf{P}}$ and $\tilde{\mathbf{P}}^*$ are complex macroscopic polarization and its complex conjugate respectively. Note that

$$2n\eta Re(\sigma_{21}e^{-i\omega t}) = 2Re(\tilde{\mathbf{P}}e^{-i\omega t}). \quad (2.47)$$

At this moment we found out how to relate coherences to electromagnetic quantities [6]. Let us write down the relation $\tilde{\mathbf{P}} = \tilde{\mathbf{P}}(\sigma_{21})$ and then continue to modify the Bloch equations (2.38) – (2.40):

$$\tilde{\mathbf{P}} = n\eta\sigma_{21}. \quad (2.48)$$

Simply by inserting equations (2.8) and (2.48) into (2.40) we obtain

$$\frac{1}{n\eta} \frac{d\tilde{\mathbf{P}}}{dt} = -(\Gamma - i\delta) \frac{\tilde{\mathbf{P}}}{n\eta} - \frac{i}{\hbar} \eta \mathbf{A}(\rho_{22} - \rho_{11}). \quad (2.49)$$

Now, we just multiply it by $n\eta$ to get

$$\frac{d\tilde{\mathbf{P}}}{dt} = -(\Gamma - i\delta)\tilde{\mathbf{P}} - i\frac{\eta^2 \mathbf{A}}{\hbar}(\rho_{22} - \rho_{11})n. \quad (2.50)$$

It would be meaningful to avoid variables ρ_{22} and ρ_{11} . Let us analyze term $(\rho_{22} - \rho_{11})n$. To find its meaning we expand it

$$(\rho_{22} - \rho_{11})n = \rho_{22}n - \rho_{11}n = |c_2|^2 n - |c_1|^2 n. \quad (2.51)$$

We see that it is the probability of measuring state $|2\rangle$ times number of atomic systems per unit volume minus the probability of measuring state $|1\rangle$ times number of atomic systems per unit volume. It is not an overestimation to say that n is a very large number. For this reason, we may say that it is the difference of number of atomic systems in state $|2\rangle$ and $|1\rangle$ respectively at a given time. In the laser community it is called the population inversion [4, 6]. So, we define it in case of two-level system as

$$\Delta n = (\rho_{22} - \rho_{11})n. \quad (2.52)$$

Equation (2.50) then becomes

$$\frac{d\tilde{\mathbf{P}}}{dt} = -(\Gamma - i\delta)\tilde{\mathbf{P}} - i\frac{\eta^2}{\hbar}\mathbf{A}\Delta n. \quad (2.53)$$

This is the first of **the Maxwell-Bloch equations** [6]. Sometimes they are called optical Bloch equations. They couple together population inversion, complex amplitude and complex macroscopic polarization. We will discuss their meaning and applications in laser physics later.

It should be mentioned that it can be shown using similar reasoning that population inversion must be greater than zero in laser to achieve amplification. One just has to calculate a susceptibility and use connection between atomic polarization and coherences. Then, it should be assumed that laser is in a so-called **steady-state**. There is a very large class of lasers that are working in a continuous regime. It means that when we turn it on, after a certain interval of time laser will achieve state in which population inversion, complex amplitude and macroscopic polarization are constant in time. That state is called steady-state. We would find susceptibility as a function of population inversion [6]. Finally, if we obtained solution of Helmholtz equation with a given susceptibility we would see that if

- $\Delta n = 0$: laser medium would be transparent for incoming light.
- $\Delta n > 0$: the light would be amplified and lasing would be possible.
- $\Delta n < 0$: the active medium would absorb light.

Before we continue to present the derivation of next Maxwell-Bloch equations, we will make a short comment on a three and four-level quantum systems.

2.3.2 More realistic atomic systems

Until now, we were analyzing basic interactions in lasers using very simple idealized two-level atomic systems. As far as we know two-level lasing systems does not exist or they are extremely rare and they would be/are very impractical. It is for example impossible to achieve population inversion in two-level system by optical pumping [1]. In this part we want to discuss more realistic and complex atomic systems used in real lasers. Most lasers are based on **three-level** and **four-level** atomic systems.

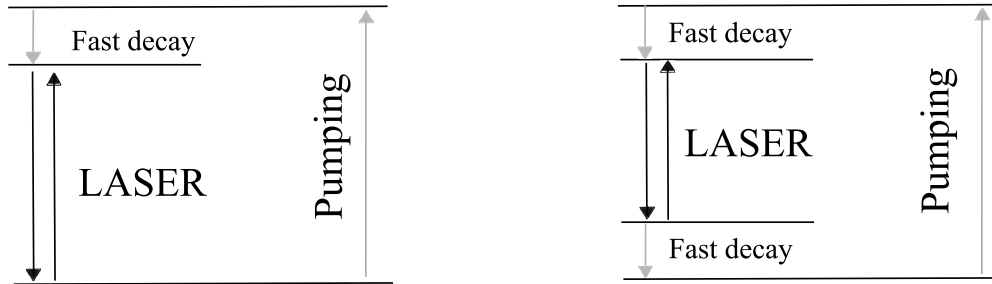


Figure 2.2: *Three - level system on the left and four-level lasing system on the right.*

Let us first discuss a three-level case (see Figure 2.2). Such system consists of three energy levels: $|0\rangle$, $|1\rangle$ and $|2\rangle$. We used $|0\rangle$ instead of $|1\rangle$ in case of the lowest level to suggest that it is a ground-level. The lasing is going on thanks to transitions between $|0\rangle$ and $|1\rangle$. On the other side, the pump (it is not important what mechanism is responsible for pumping) excites atomic systems from the ground-state directly to state $|2\rangle$ which is usually short-lived. It means that it immediately decays and number of atomic systems per unit volume in state $|2\rangle$ can be approximated as zero. Probably the most famous three-level laser is Maiman's original laser [6].

Energy levels of four-level systems are then $|0\rangle$, $|1\rangle$, $|2\rangle$ and $|3\rangle$. Similarly as in the three-level case the pump excites atomic systems from the ground-state to state $|3\rangle$. Laser is based on transitions between states $|1\rangle$ and $|2\rangle$. Here, short-lived states are $|1\rangle$ and $|3\rangle$. It is very interesting because if $n_1 \cong 0$ then $\Delta n = n_2 - n_1 \cong n_2$. That is very important aspect of four-level systems and it was mentioned because we will use it in derivation of next Maxwell-Bloch equations [1, 6].

Someone could say that all previously presented derivations based on two-level systems does not make sense and the reasoning lacks generality. However, as we have seen for example in case of the rotating-wave approximation, we can suspect that the light-matter interactions such as stimulated emission have very sharp resonance curve [1]. It means that transitions that significantly differ from each other from a point of view of their energies are very slightly influenced by each other. For this reason we may study only that parts of three or more-level systems that are responsible for laser light emission. Only influences that we take into account are populations decays which can be built-in phenomenologically. It has at least one more consequence. If we derived equations describing dynamics of for example four-level

laser we would be able to modify them easily so that they would describe three-level laser. We will use four-level laser scheme in the next derivations for simplicity [6, 1].

2.3.3 Complete Maxwell-Bloch equations

Let us now continue the derivation of Maxwell - Bloch equations. In the previous section, we saw that in the typical four-level laser $\Delta n \cong n_2$. After multiplication of Equation (2.39) using n , it becomes

$$n \frac{d\rho_{22}}{dt} = \frac{d}{dt}(n\rho_{22}) = n\Lambda_2 - \gamma_2 n\rho_{22} - \frac{i}{2}n(\omega_R^* \sigma_{21} - \omega_R \sigma_{21}^*). \quad (2.54)$$

Next, if $\Delta n \cong n_2$ we have

$$\frac{d\Delta n}{dt} = W - \gamma\Delta n - \frac{i}{2}n(\omega_R^* \sigma_{21} - \omega_R \sigma_{21}^*), \quad (2.55)$$

where $W = n\Lambda_2$ denotes to the pumping rate. Additionally, we know that $\omega_R = \omega_R(\mathbf{A})$ and $\sigma_{21} = \sigma_{21}(\tilde{\mathbf{P}})$. Let us insert Equations (2.8) and (2.48) into Equation (2.55) and write that

$$\frac{d\Delta n}{dt} = W - \gamma\Delta n - \frac{i}{2}n\left(\frac{2\eta\mathbf{A}^*}{\hbar}\frac{\tilde{\mathbf{P}}}{n\eta} - \frac{2\eta\mathbf{A}}{\hbar}\frac{\tilde{\mathbf{P}}^*}{n\eta}\right), \quad (2.56)$$

in which we can cancel n and η . After doing so, we finally obtain the second Maxwell-Bloch equation:

$$\frac{d\Delta n}{dt} = W - \frac{\Delta n}{\tau} - \frac{i}{\hbar}(\mathbf{A}^*\tilde{\mathbf{P}} - \mathbf{A}\tilde{\mathbf{P}}^*). \quad (2.57)$$

Note that $\gamma = \frac{1}{\tau}$, where τ is often called **the population inversion lifetime**.

It should be mentioned that very often the pumping rate is written as $\frac{\Delta n_0}{\tau}$, where Δn_0 is called **the unsaturated population inversion**. The physical interpretation is not clear at first sight. However, we can show its interpretation using the following reasoning. Imagine that there is no electric field in resonant cavity (no laser emission, in fact) and we are trying to find steady - state solution of population inversion. Then, we can write that

$$\frac{d\Delta n}{dt} = 0 = W - \frac{\Delta n}{\tau} = \frac{\Delta n_0}{\tau} - \frac{\Delta n}{\tau} \Rightarrow \Delta n = \Delta n_0.$$

It can be shown in many ways that generally the steady-state solution of population inversion depends on amplitude of electric field inside cavity. We can say that electric field saturates population inversion. Given situation is a lot easier to imagine if we think of light as particles - photons. The more photons there is the more probable stimulated emission is. Then, when we assume that $\Delta n > 0 \Leftrightarrow n_2 > n_1$ the population inversion will be small in case of high intensity of light. Finally we can interpret Δn_0 by saying that it is population inversion in steady - state when laser is not working and pumping rate is equal to $\frac{\Delta n_0}{\tau}$ [1]. The second Maxwell - Bloch equation then reads

$$\frac{d\Delta n}{dt} = \frac{\Delta n_0}{\tau} - \frac{\Delta n}{\tau} - \frac{i}{\hbar}(\mathbf{A}^*\tilde{\mathbf{P}} - \mathbf{A}\tilde{\mathbf{P}}^*). \quad (2.58)$$

The last Maxwell-Bloch equation we have to obtain is equation of complex amplitude's time-evolution. In order to describe evolution of electric fields inside resonant cavity with active medium we should derive modified wave equation. Modified in this way that it will contain macroscopic polarization. We begin with writing down two Maxwell equations we need:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} = -\frac{1}{v} \frac{\partial \mathbf{E}}{\partial t}, \quad \nabla \times \mathbf{H} = \varsigma \mathbf{E} + \frac{\partial \mathbf{D}}{\partial t}, \quad (2.59)$$

where \mathbf{B} is vector of magnetic induction, \mathbf{D} is electric displacement vector, \mathbf{H} is magnetic field intensity vector and v is velocity of light in medium with refractive index n_0 . Here, we assumed that there are no other nonlinear effects than amplification and no anisotropies. Relation $\mathbf{E} = v\mathbf{B}$ was used. In the second equation there was introduced fictive conductivity because in every cavity there are some losses of energy. These losses can be modeled using fictive conductivity ς [6]. Let us now use mathematical definition of electric displacement vector and multiply the second equation using rotation operator:

$$\nabla \times \nabla \times \mathbf{H} = -\nabla^2 \mathbf{H} = \varsigma \nabla \times \mathbf{E} + \epsilon_0 \frac{\partial}{\partial t} \nabla \times \mathbf{E} + \frac{\partial}{\partial t} \nabla \times \mathbf{P}, \quad (2.60)$$

where ϵ_0 is permittivity of vacuum. At this point we do not know what is $\nabla \times \mathbf{P}$ equal to. In the linear approximation it can be easily calculated.

$$\nabla \times \mathbf{P} = \nabla \times (\epsilon_0 \chi \mathbf{E}) = \epsilon_0 \chi \nabla \times \mathbf{E} = -\frac{\epsilon_0 \chi}{v} \frac{\partial \mathbf{E}}{\partial t} = -\frac{1}{v} \frac{\partial \mathbf{P}}{\partial t}. \quad (2.61)$$

χ is susceptibility. After doing that the equation becomes

$$\begin{aligned} \frac{1}{\mu v} \nabla^2 \mathbf{E} - \frac{\varsigma}{v} \frac{\partial \mathbf{E}}{\partial t} - \frac{\epsilon_0}{v} \frac{\partial^2 \mathbf{E}}{\partial t^2} &= \frac{1}{v} \frac{\partial^2 \mathbf{P}}{\partial t^2}, \\ \Downarrow \\ \nabla^2 \mathbf{E} - \epsilon_0 \mu \frac{\partial^2 \mathbf{E}}{\partial t^2} - \varsigma \mu \frac{\partial \mathbf{E}}{\partial t} &= \mu \frac{\partial^2 \mathbf{P}}{\partial t^2}. \end{aligned} \quad (2.62)$$

Electric field intensity and electric dipole density in the laser cavity must obey this equation. The next step is to put needed quantities into it. This can be done by writing

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{A}^*(\mathbf{r}, t) e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} + c.c., \quad \mathbf{P}(\mathbf{r}, t) = \tilde{\mathbf{P}}^*(\mathbf{r}, t) e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} + c.c., \quad (2.63)$$

where *c.c.* stands for complex conjugate. It can be seen directly even before inserting it into wave equation that result would be impractically big equation and we will not write it here. Instead of this, we can say that if losses and gain in the cavity are weak we can use **slowly varying amplitude approximation** and neglect most of the terms [6]. For example all the second time derivatives or derivatives with respect to spatial variables because they are very small compared to for example $\frac{d\mathbf{A}}{dt}$. We should mention that there is a symmetry and the dynamics of \mathbf{A} and $\tilde{\mathbf{P}}$ is the same as in the case of their conjugate counterparts. After performing all modifications and assuming that wave vector has only z -component we achieve

$$2i\epsilon_0\mu\omega \frac{\partial \mathbf{A}}{\partial t} + i\varsigma\mu\omega \mathbf{A} = -\mu\omega^2 \tilde{\mathbf{P}}. \quad (2.64)$$

We may cancel permeability and angular frequency and divide entire equation by $2i\epsilon_0$ so that we have

$$\frac{\partial \mathbf{A}}{\partial t} = -\frac{\varsigma}{2\epsilon_0} \mathbf{A} + i\frac{\omega}{2\epsilon_0} \tilde{\mathbf{P}} \quad (2.65)$$

Now, take a look at the first term on the right side of the equation. It represents losses per unit of time. Let us introduce $\tau_{ph} = \frac{\epsilon_0}{\varsigma}$ which is called **photon lifetime** of given cavity. In the first obtained Maxwell-Bloch equation there was introduced so-called detuning frequency. Here, it can be done in the similar manner. We define $\delta_{cav} = \omega - \omega_q$ to be cavity detuning frequency. All previous derivations were done for very simple Fabry-Pérot-like resonant cavity. It is clear that structure of resonator defines resonant frequencies. It means that only certain frequencies will create standing-waves in resonator. Set of resonant frequencies ω in simple resonator of length L and active medium's refractive index n_0 can be obtained in the following way. Let us write down phase condition for resonance

$$2kL = 4\frac{\pi}{\lambda_q}L = 2\pi q \Rightarrow \omega_q = \frac{\pi c}{n_0 L}q, \quad (2.66)$$

where q is an integer and c is velocity of light in vacuum. The Maxwell-Bloch equation for complex amplitude becomes

$$\frac{d\mathbf{A}}{dt} = -\frac{1}{2\tau_{ph}} \mathbf{A} + i\delta_{cav} \mathbf{A} + i\frac{\omega}{2\epsilon_0} \tilde{\mathbf{P}}. \quad (2.67)$$

This is the last of the Maxwell-Bloch equations [6]. We know that first two terms on the right side of Equation (2.67) represent influence of cavity. Losses due to absorptions or due to the fact that values of reflectivity coefficients of cavity mirrors are smaller than one and consequently an amount of photons is radiated out of the cavity. The last term represents amplification and if we recall that $\tilde{\mathbf{P}} = n\eta\sigma_{21}$ we can say that atomic coherences that induce material polarization are responsible for stimulated emission [6]. Let us now write down all Maxwell - Bloch equations [6]:

$$\boxed{\begin{aligned} \frac{d\tilde{\mathbf{P}}}{dt} &= -(\Gamma - i\delta)\tilde{\mathbf{P}} - i\frac{\eta^2}{\hbar} \mathbf{A}\Delta n, \\ \frac{d\Delta n}{dt} &= \frac{\Delta n_0}{\tau} - \frac{\Delta n}{\tau} - \frac{i}{\hbar}(\mathbf{A}^*\tilde{\mathbf{P}} - \mathbf{A}\tilde{\mathbf{P}}^*), \\ \frac{d\mathbf{A}}{dt} &= -\left(\frac{1}{2\tau_{ph}} - i\delta_{cav}\right) \mathbf{A} + i\frac{\omega}{2\epsilon_0} \tilde{\mathbf{P}}. \end{aligned}} \quad (2.68)$$

$$\quad (2.69)$$

$$\quad (2.70)$$

2.3.4 Laser classes

We reached to the point when we are able to analyze dynamics of important basic laser quantities. Imagine that someone built laser and wants to know what will be its dynamical properties. Suppose that we know all parameters of resonant cavity, we know what are optical transitions of active medium. Next we know even what is the pumping rate and all constants of populations relaxation. The first simple approach would be to solve numerically

Maxwell-Bloch equations. This would not be a simple task if we did not have a computer. That would be the case if we wanted to describe laser's working quantitatively. We should note that we are talking about time-evolution in the interval before laser reaches its steady-state. As it turns out, it is possible to qualitatively characterize dynamics of most of the continuously-working lasers by comparing three important constants: Γ , τ and τ_{ph} . For this purpose there was created following classification of lasers [6].

- **Class A** (τ_{ph} is larger than τ and $\frac{1}{\Gamma}$ by orders of magnitude) - In this case polarization and population inversion reach steady-state very quickly compared to amplitude. This is the reason we do not have to study the time - evolution of population inversion and polarization. Thus, we may perform so called **adiabatic elimination** of given quantities. In practice it means that we say that their derivation is equal to zero. In fact, we then obtain just one differential equation of the first order (for amplitude). Some lasers with gas active medium belong to class A. We should mention that some spin-polarized lasers that are important in this thesis can be described as class A lasers [7].
- **Class B** ($\frac{1}{\Gamma}$ is very small compared to τ and τ_{ph}) - Here, adiabatic elimination can be applied only to polarization. Two nonlinear coupled differential equations of the first order are still easier to solve than three such equations. Well-known Nd:YAG laser is a class B laser.
- **Class C** (time constants are all of the same order of magnitude) - There is no possibility of adiabatic elimination. Solution of Maxwell - Bloch equations depends very strictly on initial conditions.

2.4 The rate equations approximation

The Maxwell-Bloch equations (2.68) – (2.70) are powerful tool for analysis of laser's dynamical properties. As we could see in the derivation of them, they take into account wave-like character of light. It would have significant meaning if we wanted for example to know how laser's dynamics would change if we modified cavity length slightly. However, very often calculations using Maxwell-Bloch equations are not stable or more precisely: it is difficult to find meaningful parameters so that Maxwell-Bloch equations give results corresponding with reality. Additionally, lasers are constructed to fulfill the resonance condition. It means that in certain situations we can make **the rate equations approximation** [6]. It is based on the idea that laser dynamics can be described only by population inversion and energy (the number of photons) which is being inter-changed between active medium and photon field. The wave nature of light is neglected in this case. In this section we will make the transition from the Maxwell-Bloch equation to the rate equations which are lot easier to work with.

Next, we will show how to calculate the photon lifetime in a given resonant cavity. Finally, we will use the rate equations to compare dynamics of A and B laser classes.

2.4.1 From Maxwell-Bloch equations to rate equations

It was already stated that rate equations describe only population inversion and the number of photons in cavity. It is natural to expect that we need to adiabatically eliminate material polarization. For this reason the rate equations approximation is valid only for A and B class lasers. Let us perform adiabatic elimination [6]

$$\begin{aligned}\frac{d\mathbf{P}}{dt} &= -(\Gamma - i\delta)\tilde{\mathbf{P}} - i\frac{\eta^2}{\hbar}\mathbf{A}\Delta n = 0 \\ \Downarrow \\ \tilde{\mathbf{P}} &= -i\frac{\eta^2}{\hbar}\frac{1}{\Gamma - i\delta}\mathbf{A}\Delta n.\end{aligned}\tag{2.71}$$

If we insert term describing polarization (2.71) into Equation (2.69) we will obtain

$$\frac{d\Delta n}{dt} = -\frac{1}{\tau}(\Delta n - \Delta n_0) - \frac{1}{\tau I_{sat}}I\Delta n.\tag{2.72}$$

In this equation the **saturation intensity** (I_{sat}) was introduced. We should mention that using actual formalism it is time - consuming and not easy at all to derive what saturation intensity is equal to. Detailed derivation is presented in Ref. [1]. We already discussed the fact that the higher the light intensity inside cavity is the smaller population inversion is. The saturation intensity is defined as the intensity of light which would cause reduction of steady-state population inversion to half of its original value (when there was no light). The original value is the value which is not saturated at all or very slightly.

In the case of complex amplitude, we will proceed differently. We want to work with such quantities as light intensity or the number of photons. For this reason we should find the light intensity as a function of complex amplitude. We know that

$$I = |\mathbf{S}|_t = |\mathbf{E} \times \mathbf{H}|_t = \left| [\mathbf{A}^* e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} + c.c.] \times [\tilde{\mathbf{H}}^* e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} + c.c.] \right|_t,\tag{2.73}$$

where \mathbf{S} stands for Poynting vector, \mathbf{k} and \mathbf{r} are wavevector and position vector respectively. The index 't' denotes to time-averaging. Next, we should find relation of \mathbf{E} to \mathbf{H} . We assume that they are orthogonal:

$$\mathbf{E} = v\mathbf{B} = v\mu_0\mathbf{H} = \frac{v}{\epsilon_0 c^2}\mathbf{H} = \frac{1}{\epsilon_0 n_0 c}\mathbf{H}.\tag{2.74}$$

If we insert Eq. (2.74) into (2.73) we will obtain

$$I = \epsilon_0 n_0 c \left| 2|\mathbf{A}|^2 + (\mathbf{A}^*)^2 e^{i2(\omega t - \mathbf{k} \cdot \mathbf{r})} + (\mathbf{A})^2 e^{-i2(\omega t - \mathbf{k} \cdot \mathbf{r})} \right|_t = 2\epsilon_0 n_0 c |\mathbf{A}|^2.\tag{2.75}$$

Let us now calculate the derivative of I .

$$\frac{dI}{dt} = 2\epsilon_0 n_0 c \frac{d}{dt} |\mathbf{A}|^2 = 2\epsilon_0 n_0 c \frac{d}{dt} (\mathbf{A}^* \mathbf{A}) = 2\epsilon_0 n_0 c \left(\mathbf{A}^* \frac{d\mathbf{A}}{dt} + \mathbf{A} \frac{d\mathbf{A}^*}{dt} \right).\tag{2.76}$$

After making use of Maxwell-Bloch equation for complex amplitude (2.70) and its conjugate counterpart we have

$$\frac{dI}{dt} = \frac{1}{\tau_{ph}\Delta n_{th}} I \Delta n - \frac{I}{\tau_{ph}}. \quad (2.77)$$

Here, the situation is similar to that with population inversion, where the saturation intensity was introduced. In that equation we introduced so called **threshold population inversion** (Δn_{th}). It is the smallest possible population inversion in which laser oscillation is possible. Its value may be derived using the fact that gain and losses must be equal in order to make lasing possible. Again, it was elegantly shown in Ref. [1]. We should notice that in steady-state $\Delta n = \Delta n_{th}$. In order to make possible the next steps in derivation of the rate equations we write down values of I_{sat} and Δn_{th} .

$$I_{sat} = \frac{h\nu}{\sigma(\nu)\tau}, \quad \Delta n_{th} = \frac{n_0}{\sigma(\nu)\tau_{ph}c}. \quad (2.78)$$

In the previous relations we can find new parameter $\sigma(\nu)$. It is the cross section characterizing the probability of stimulated emission and absorption. It is used mainly in models which are working with particle-like picture of light [1, 8].

We mentioned earlier in this that the rate equations are working with the population inversion and the number of photons. That means that we have to recalculate intensity of light to the number of photons. Thus, if we assume that cavity has constant area of section S , the number of photons is equal to

$$F = \Phi S \frac{L}{v} = \frac{I}{h\nu} S \frac{n_0 L}{c} = \frac{n_0 V}{h\nu c} I, \quad \Rightarrow \quad dF = \frac{n_0 V}{h\nu c} dI, \quad (2.79)$$

where Φ is photon flux. All that we now have to do is modification of Eq. (2.72) and (2.77). Finally we obtain

$$\boxed{\begin{aligned} \frac{d\Delta N}{dt} &= \frac{\Delta N_0}{\tau} - \kappa F \Delta N - \frac{\Delta N}{\tau}, \\ \frac{dF}{dt} &= \kappa F \Delta N - \frac{F}{\tau_{ph}}. \end{aligned}} \quad (2.80)$$

$$(2.81)$$

where $\Delta N = V \Delta n$. If someone went through the entire derivation he/she would notice that

$$\kappa = \frac{c\sigma}{n_0 V}. \quad (2.82)$$

It is coefficient of stimulated emission. It can be shown very quickly how we would obtain term representing stimulated emission using probability theory arguments and cross section. Imagine that there is one photon and one excited atomic system in a cavity with section area S . The probability of stimulated emission and the probability per unit time are [1]

$$P_{11} = \frac{\sigma}{S} = \frac{\sigma}{V} z \quad \Rightarrow \quad w_{11} = \frac{d}{dt} P_{11} = \frac{\sigma}{V} \frac{dz}{dt} = \frac{c\sigma}{n_0 V}. \quad (2.83)$$

The index 11 means one photon and one atomic system. Next, imagine that there are ΔN excited atomic systems. We may expect that the probability of stimulated emission would

be ΔN - times higher. It should be mentioned that it is not probability, it is rather rate of a given process:

$$w_{1\Delta N} = \Delta N w_{11} = \frac{c\sigma}{n_0 V} \Delta N = \kappa \Delta N. \quad (2.84)$$

Usually in cavity there is not just one photon. Thus, let us assume now that there are F photons and ΔN excited atomic systems. The rate would be in this case

$$w_{F\Delta N} = F w_{1\Delta N} = \frac{c\sigma}{n_0 V} F \Delta N = \kappa F \Delta N. \quad (2.85)$$

We obtained term describing stimulated emission on few lines without need of quantum-mechanical calculations. This is the power of typical mechanisms of construction of the rate equations although it has certain disadvantages.

Let us now discuss the meaning of each term in the rate equations. First, let us analyze equation describing population inversion. The first term represents pumping. The second one describes stimulated emission. It is worth to notice that the same term is in the second rate equation too but with opposite sign. The interpretation of this is very simple. The simplicity lays in the fact that we work with particle-like picture of light now. If the single photon was created the population inversion would change by one because one atomic system would get de-excited. The last term is just manifestation of the fact that levels in atom have finite lifetimes. This term may include for example **the spontaneous emission**. Finally, we take a look at the equation describing dynamics of the number of photons. We now that the first term represents stimulated emission and the second is responsible for losses due to not ideal mirrors of cavity or additional absorptions in active medium. the spontaneous emission was not included in this equation because we assume that it has not major effects on lasing process.

As we see the rate equations are very easy to understand and to construct. We just have to include all important processes and know how to write down their rates. Recall now that we did all previous derivations for so called four-level systems where the lower level is approximately empty. In the three-level case there would be at least one difference. The lower level is not empty and it should be taken into account. Let us have the three-level system and analyze stimulated emission of one photon. Populations of two levels between which laser works are originally for example (N_2, N_1) . When the photon is created populations will change in the following way: $(N_2 - 1, N_1 + 1)$. The population inversion was originally $\Delta N_i = N_2 - N_1$. After stimulated emission it is $\Delta N_f = N_2 - N_1 - 2 = N_i - 2$. It means that in the typical three-level system the creation of one photon equals to change of population inversion by 2. The population inversion rate equation for three-level systems then becomes [6, 1]

$$\frac{d\Delta N}{dt} = \frac{\Delta N_0}{\tau} - 2\kappa F \Delta N - \frac{\Delta N}{\tau}. \quad (2.86)$$

2.4.2 Calculation of τ_{ph} in case of a simple cavity

Let us consider a simple resonant cavity of length L with mirrors of reflection coefficients R_1 and R_2 . Let us assume that there are additional losses caused by absorptions in active medium. The active medium does not have to be fully homogenous. It can be composed of several types of atoms and lasing is possible only thanks to one certain type of atom. There may be elements that absorb light of wavelength on which laser operates, for example metals. Additional absorptions may be represented using absorption coefficient α_a . Let us assume that the intensity of light inside passive cavity is for example I_0 at a certain time t_0 . We want to know how the intensity will change if light goes through the entire resonator. It means that it reflects on both mirrors and travel the distance $2L$. The intensity I will be [1]

$$I = R_1 R_2 I_0 e^{-2\alpha_a L}. \quad (2.87)$$

The left side of equation can be modified if we use effective absorption coefficient α_e in the following way:

$$I = I_0 e^{-2\alpha_e L} = R_1 R_2 I_0 e^{-2\alpha_a L}. \quad (2.88)$$

After performing simple operations we have for α_e :

$$\alpha_e = \frac{1}{2L} \ln \frac{1}{R_1 R_2} + \alpha_a. \quad (2.89)$$

However, we wanted to obtain time constant. To do this, we should introduce time of one round trip t_{RT} which is equal to $t_{RT} = \frac{2n_0 L}{c}$. Let us use it and write

$$e^{-2\alpha_e L} = e^{-\frac{\alpha_e c}{n_0} t_{RT}} = e^{-\frac{t_{RT}}{\tau_{ph}}}. \quad (2.90)$$

By comparing sides of equation we see that [1]

$$\tau_{ph} = \frac{n_0}{\alpha_e c}. \quad (2.91)$$

It is very important to mention that it is not general method of τ_{ph} calculation. Later, we will analyze complex resonating structures for which this approach is not applicable. This issue will be discussed in the next chapters.

2.4.3 The transient behavior comparison of different laser classes

In this part we will make a use of the rate equations and we will show what is the behavior of class A and class B lasers before they reach steady-state. Note that we can compare only A and B lasers because in case of class C lasers it is not possible to eliminate adiabatically polarization and use the rate equations approximation.

We begin with class B lasers. It should be mentioned that the number of photons is normalized so that in steady - state it is equal to one. However, it does not change qualitative information about laser's dynamics. We see in the Figure 2.3 that class B laser produces

something similar to light pulses before it reaches steady-state. It is caused by the fact that τ is larger than τ_{ph} . It means that photon loss rate is much higher than de-excitation rate of excited states. It takes longer to start generating photons because of high cavity losses and relatively high lifetime of excited states. However, when laser reaches high value of population inversion even the small amount of photons will cause very fast de-population. This causes "the chain reaction" and lots of photons are created. Because of small photon lifetime they are quickly absorbed or radiated out of the laser cavity.

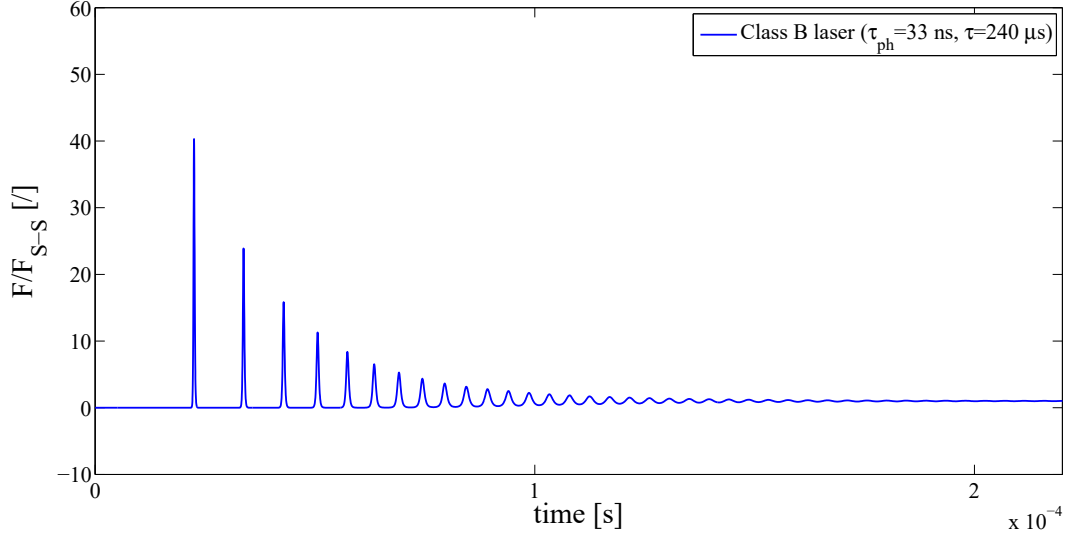


Figure 2.3: *Time-dependence of normalized number of photons in case of class B laser. F_{S-S} is the number of photons in steady-state*

This process repeats periodically until laser reaches steady-state. It should be noted that there are methods working on similar principle in order to generate laser pulses. Let us mention for example so called Q-switching [6, 1, 8]. Such laser is pumped and α_e of cavity is artificially kept very high. Then α_e is at certain moment lowered to very small value. It means that very high value of Q-factor (quality factor) of cavity is obtained (this is the reason why it is called Q-switching). This causes "the chain reaction" and very large number of photons is created in very short time interval.

On the other side, class A lasers have higher photon lifetime than that of upper population. For this reason the laser oscillation starts very quickly because it does not have to reach high value of population inversion. We can see the evolution of normalized number of photons of class A laser in Figure 2.4.

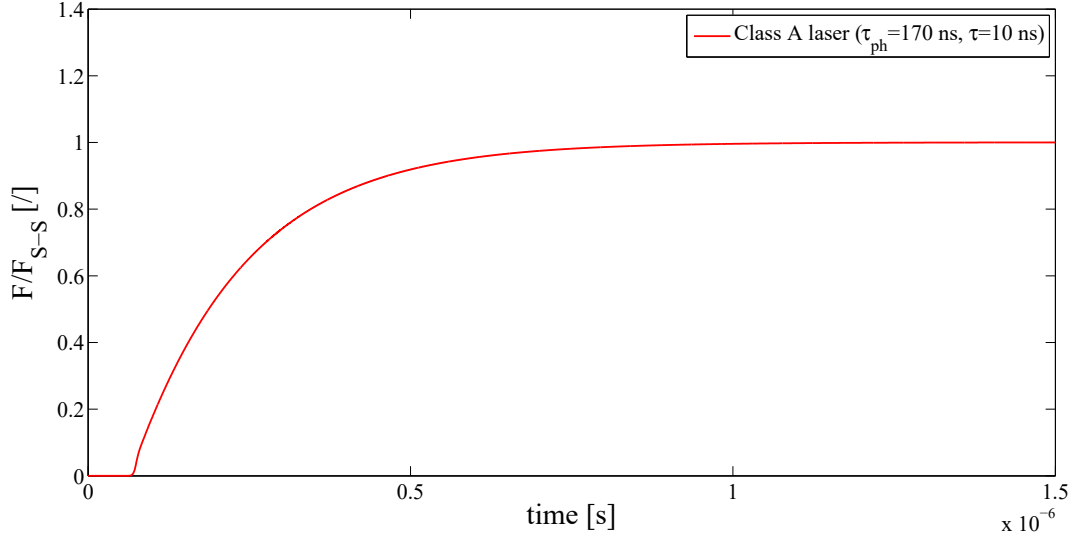


Figure 2.4: *Time - dependence of normalized number of photons in case of class A laser.*

Finally, we wanted to show (see Figure 2.5) that when we are changing lifetime parameters from those of class B to class A through certain inter-states then we observe that the transition from B to A is elegantly continuous. We see that class A laser reaches its steady-state very quickly which is not the general fact, however. The first pulse of typical class B laser does not even belong to time interval we studied.

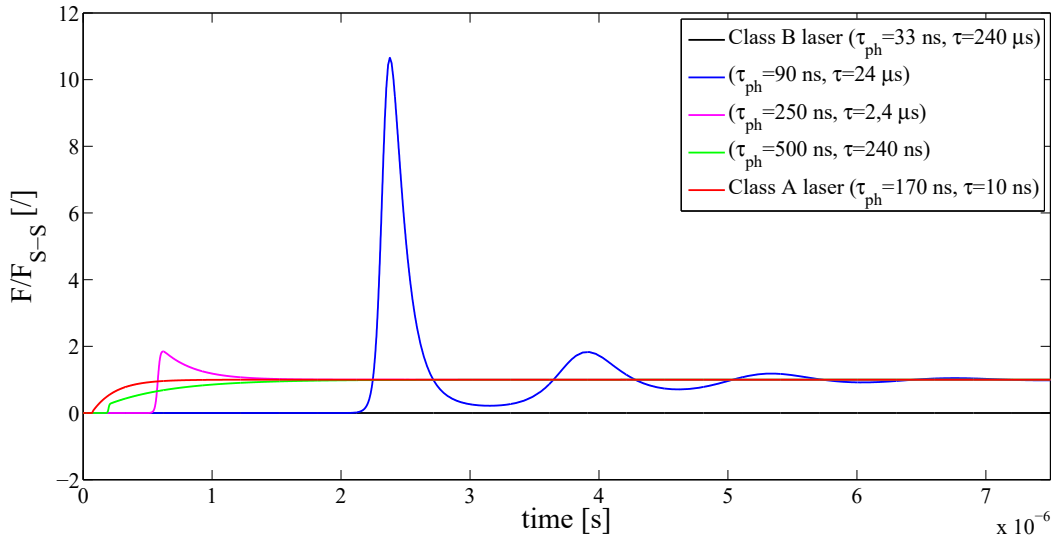


Figure 2.5: *The comparison of time - evolution of normalized number of photons of five different lasers. We begin with class B laser and then we change lifetimes to obtain typical class A laser.*

Chapter 3

Spin - polarized lasers

In the previous chapter we presented basic issues of laser physics and the light-matter interactions. All the derivations were done for general amplifying medium which was placed in a very simple resonant cavity. It should be noted that we considered only single mode lasers. In this chapter we want to discuss one particular class of laser devices: spin-polarized lasers (spin-lasers). The concept of spin-optoelectronics arised from the spintronic research. Spintronics is the field in which spin of electron or other particles is used to carry the information. It may be compared to electronics where the carriers of information are charges of electrons or holes [19]. Spin is the fundamental quantum-mechanical property of elementary particles. In fact, it is an intrinsic angular momentum. However, it should be understood only as an analogy. In order to rigorously explain a spin, we would have to use a framework of relativistic quantum mechanics, which is beyond the scope of this thesis. We are limited to the use of non-relativistic quantum mechanics to which spin was built-in artificially. Spin-optoelectronic devices benefit from the fact that the total angular momentum of photons can be directly related to their electromagnetic polarization [19, 14]. Resulting polarization state of emitted photon depends on particular transitions in active medium. This and a lot more will be discusses and analyzed in the following chapter.

3.1 The overview

Before we start to study for example spin-laser's resonant cavities or optical transitions precisely, we will describe basic spin-laser's principles in a simplified way in order to get into the picture. Spin-lasers we are studying posses so called VCSEL-geometry. It was mentioned in Introduction that VCSEL stands for **V**ertical-**C**avity **S**urface-**E**mitting **L**aser. Today, VCSEL is a well-known technology with numerous applications in data storage or in optical communications. VCSELs are semiconductor lasers in which a resonant cavity consists of two Bragg reflectors. Such reflectors consist of dielectric thin layers. The Bragg reflectors have very high reflectivity for certain interval of wavelengths of light. Semiconductor lasers are pumped by electric current or optically [19]. Since they are made of semiconductor

crystals, electrons concentrate in a conduction band. When the electron re-combines with a valence band hole, the photon is created as a consequence of energy conservation. The next essential components of VCSELs are the quantum wells. The quantum well is a region with lower energy potential than its surroundings. In practice, we can create the quantum well by placing thin layer of material with certain band gap between materials with larger band gap. When we write "semiconductor band gap" we mean energy difference between a conduction and a valence band. Despite the fact that we have to use quantum mechanics to describe the quantum wells completely, we can expect even from the classical point of view that conduction band electrons may "fall" into the wells. The possible energies of electrons in the quantum wells are discrete in a case of bound states. By changing a width of the well we can optimize electron's possible energies and consequently approximate energies of emitted photons. VCSEL's active medium is formed by multiple quantum wells that are placed between two Bragg reflectors.

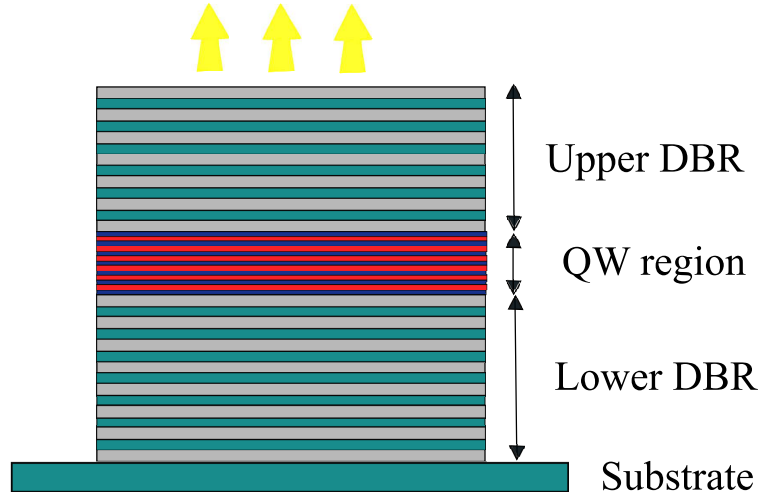


Figure 3.1: *A simplified scheme of VCSEL geometry.*

We can start talking about spin-VCSELs when we pump VCSEL using electrons with certain spin polarization or optical pumping with preferred circular polarization. Electron spin polarization is defined as [14, 19]

$$P_n = \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}}, \quad (3.1)$$

where n_{\uparrow} and n_{\downarrow} are electron concentrations with spin-up and spin-down. Spin-up means that the projection of electron's spin on certain axis (which is chosen by us) is positive. In case of electrons in a conduction band spin is their total angular momentum. We can associate total angular momentum and its projection on certain axis even to hole bands. It turns out that only some transitions are possible due to the selection rules [19, 14]. The angular momentum of emitted photon depends strictly on combination of angular momenta projections of electron and hole band the electron re-combines with. Now it may be clear why the electron spin polarization is important. We noted that angular momentum of photon is

connected to its electromagnetic polarization. Thus, by changing electron spin polarization we should be able to control polarization of emitted light. As we are going to see it is not that simple. Additionally, spin-VCSELs may contain parts which polarize electron spins. It is possible thanks to a spin-injector which consists of combination of magnetized metallic layers [19, 14].

3.2 VCSEL's resonant cavity

In this section we describe basic properties of Bragg reflectors, which forms spin-VCSEL's resonant cavity. Ellipsometric measurement of GaAs/AlAs Bragg mirror will be presented as well.

3.2.1 Distributed Bragg reflectors

As we mentioned previously, the gain region of VCSEL structures is small and very high reflectivity coefficients of resonator's mirrors are needed. For this reason for example conventional metallic mirrors are not suitable. DBR (**D**istributed **B**ragg **R**eflectors) consist of multiple dielectric thin layers, very often thin layers, of different refractive indexes and thicknesses. These two properties may be distributed periodically in DBR. If the number of periods of some set of layers is large enough we can observe existence of photonic band gap [3]. It is similar as in case of solids, where electrons cannot have energies of certain values. The existence of photonic band gap in such structure manifests itself as nearly perfectly reflecting. In practice, however, reflectivity coefficients for band gap wavelengths may be very close to one. There is always the evanescent wave which penetrates through entire structure.

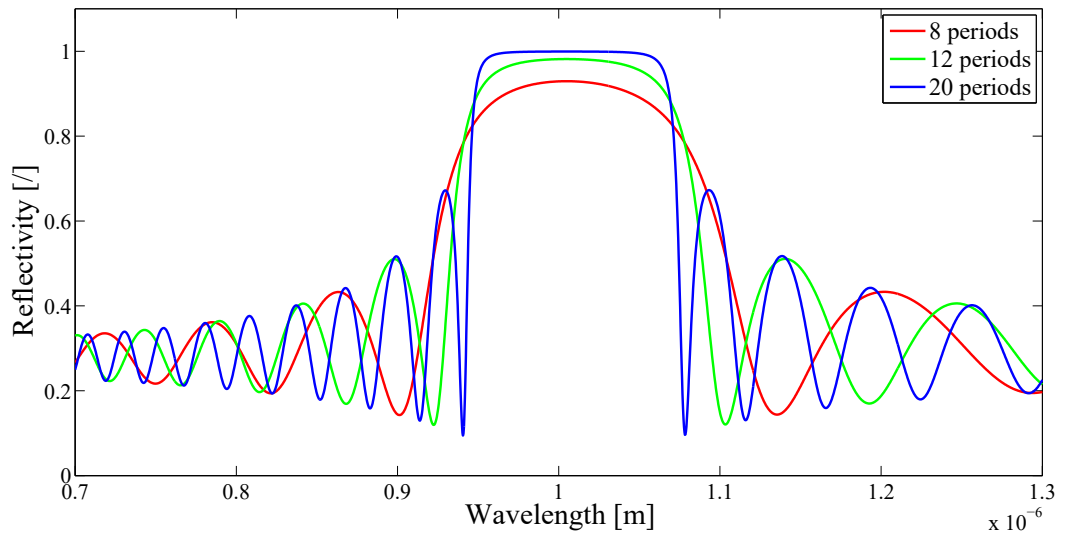


Figure 3.2: *The comparison of the Bragg reflectors with different numbers of GaAs/AlAs periods.*

We calculated the spectral response of DBR with different numbers of periods of GaAs/AlAs on GaAs substrate (see Figure 3.2). It may be observed that more periods there are the sharper band gap and higher reflectivity coefficient we get. We used matrix formalism presented in Appendix B. The parameters of layers were based on the ellipsometric measurement that will be presented below.

Since the thicknesses of layers in DBR are very small, sophisticated methods must be used to fabricate them. Probably the best known technique of thin films growth is the MBE (**M**olecular **B**eam **E**pitaxy) [3]. It is possible to grow films one atomic layer after layer. Moreover, there must be achieved very-high vacuum in the MBE chamber.

3.2.2 Experimental part-ellipsometric measurement of DBR

Spectroscopic ellipsometry is optical technique that can be used to measure thickness of thin films, optical functions of materials and a lot more. In order to analyze such physical quantities it measures changes in polarization of light. They are described by so called ellipsometric angles Ψ and Δ , which are defined as [23, 28]

$$\frac{r_p}{r_s} = \operatorname{tg}\Psi \cdot e^{i\Delta}, \quad (3.2)$$

where r_p and r_s are the amplitude reflectivity coefficients for p- and s- polarizations. The disadvantage of the ellipsometry is that when we measure for example multilayered structure, we have to create a model to extract informations about constituents of structure from measured data.

The next important ability of ellipsometry is to measure Mueller matrix. Polarization state of light can be described by Stokes vectors, that are defined in the following way [3]:

$$\mathbf{S} = \begin{pmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{pmatrix}, \quad (3.3)$$

where S_0 is the intensity of light, S_1 is the difference of intensities of linear polarizations at 0° and 90° . S_2 is the difference of intensities of linear polarizations at 45° and -45° and finally S_3 is the difference of intensities of right - circular and left - circular polarizations. If light described by \mathbf{S}_i passes through or reflects on certain optical element, its Stokes vector transforms into \mathbf{S}_f . The matrix of such transformation is the Mueller matrix, which is characteristic to each optical element. We can write [23, 28]

$$\mathbf{S}_f = \mathbf{M}\mathbf{S}_i. \quad (3.4)$$

The measurement was performed using ellipsometer Woollam RC2. A scheme of this ellipsometer is shown in Figure 3.3. It consists of light source which is deuterium-halogen lamp

in this case. Emitted light goes through linear polarizer, then through rotating compensator which is in fact a retarder. Rotating compensator modulates the signal. Light reflects on sample and goes through rotating compensator and analyzer respectively. Finally it reaches detector and signal is analyzed. It is possible to measure with fixed angle θ or changing θ .

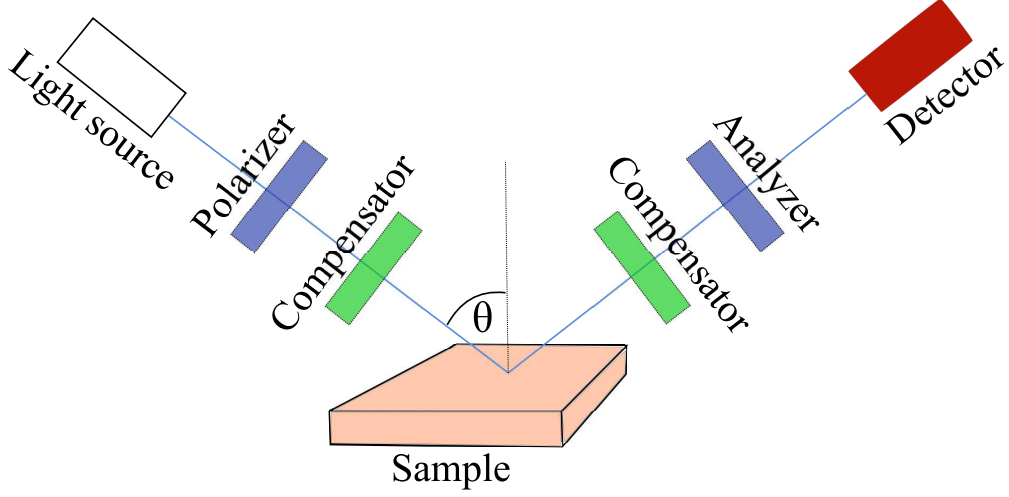


Figure 3.3: *Scheme of ellipsometer.*

Spectral range of used ellipsometer is 193 nm to 1700 nm. When we measure the reflection, range of θ is from 19° to 85° .

Data analysis was performed in CompleteEASE software. Obtained data must be compared to theoretical model which is created for example using Yeh's matrix formalism [24]. Then we perform optimization of model in order to find the best match with experiment. It can be done using Levenberg-Marquardt least-square algorithm [28]. Function used in finding of extreme depends on quantity we want to analyze. In fact we are trying to find minimal square of difference of measured quantity and calculated quantity. Let us consider that we are trying to find thickness of a thin film. We measure for example spectral dependence of reflectivity and then we calculate it. Thickness (d) is a variable during the calculation. Then we introduce a function χ which is

$$\chi^2(d, \lambda) = |R^m(\lambda) - R^c(d, \lambda)|^2, \quad (3.5)$$

where R^m is measured reflectivity and R^c is calculated reflectivity. We have to find such d for which χ^2 has minimal value. This is a simplified explanation and the procedure is called fitting procedure.

We chose to present the measurement of ellipsometric angles as a functions of the wavelength. Ψ contains information about amplitude of reflected light. In Figure 3.4 we observe a typical Bragg band gap at the center. When we look at the region of shorter wavelengths we see that measured structure absorbs light of such wavelengths. On the other side, in case of larger wavelengths there is the interference pattern.

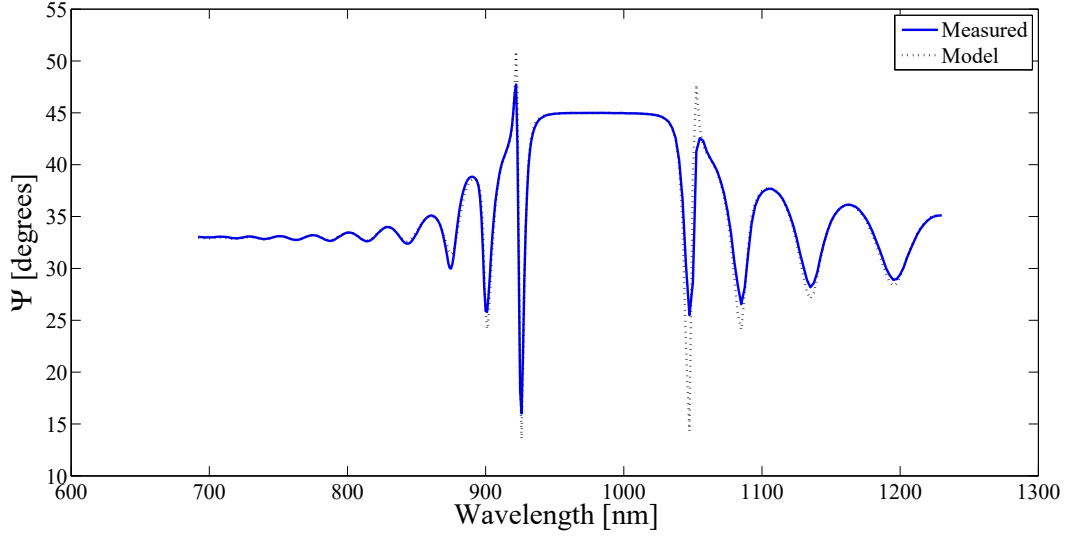


Figure 3.4: *Measured ellipsometric angle Ψ for DBR with 20 GaAs/AlAs periods compared to the model. The angle of incidence is 45° .*

Let us take a look on Figure 3.5. DBR are designed very often in the way that the wavelength of laser is at the center of a band gap [10]. Suppose that gain medium is placed between two DBR that we measured. We see that the phase shift approximately at the center of a band gap is 180° . Light of that wavelength would fulfill the resonance condition because after traveling back and forth it would have the same phase shift. However, the influence of the gain medium must be taken into account.

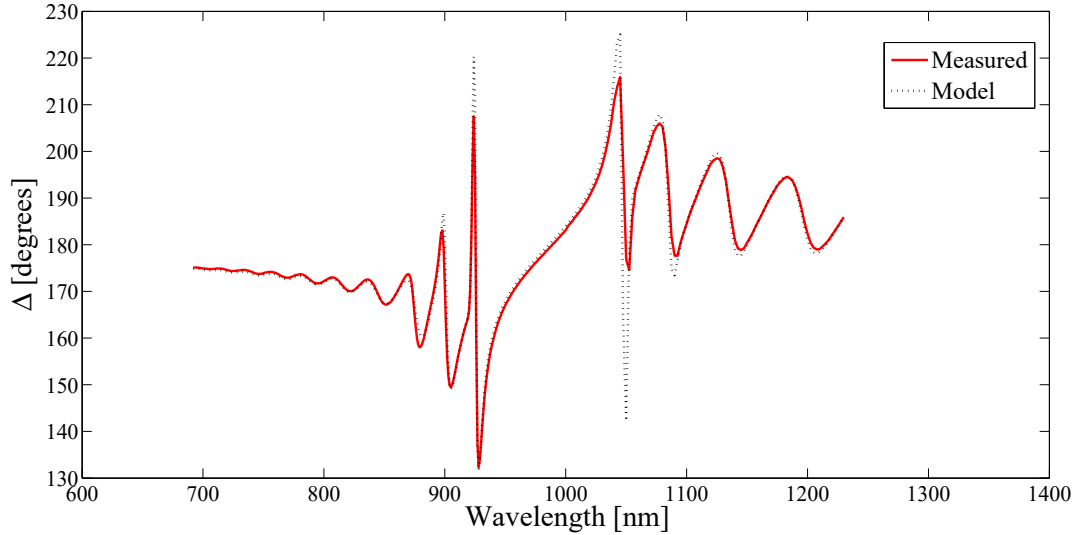


Figure 3.5: *Measured ellipsometric angle Δ for DBR with 20 GaAs/AlAs periods compared to the model. The angle of incidence is 45° .*

Thickness of AlAs layers was found using fit and is 85.08 nm. In the case of GaAs it is 71.9 nm. Additionally, we included a surface roughness by a fitting procedure and it turned out to be 4.26 nm.

3.3 Optical transitions in semiconductor crystals

The wavelengths and polarization states of laser modes are defined not only by properties of resonant cavity, but mainly by microscopic structure of active medium and possible optical transitions that can happen in it [1]. In the following section we will present what are possible states of electrons and holes in semiconductor crystals and why emitted photons are circularly polarized.

3.3.1 The amplitudes of valence and conduction band's wave functions

Since semiconductors have crystalline structure we want to know how electrons behave in periodic potential. In the year 1928 Felix Bloch formulated one of the first quantum theories of solids in his doctoral thesis. He proved that if we place a particle in periodic potential its wave function will be a plane wave with amplitude that has the same periodicity as a given potential [9]. We can write it down as

$$\psi_m(\mathbf{k}, \mathbf{r}) = u_m e^{i\mathbf{k} \cdot \mathbf{r}} \quad (3.6)$$

Where u_m is the amplitude of the wave function, \mathbf{k} and \mathbf{r} are the wavevector and position vector respectively as in the previous chapter. In order find amplitudes of possible states we have to find eigenvectors of system's Hamiltonian. Let us neglect the influence of a quantum well for a while, it is not important at the moment and its influence may be included phenomenologically. The Hamiltonian consists of isolated atom's potential Hamiltonian, the crystal potential Hamiltonian and finally, which is very important for us: spin-orbit interaction Hamiltonian [9]. Spin-orbit interaction is caused by the interaction of electron's spin with magnetic field that is generated by the electron itself, or to be more precise, by its orbital motion. There are no trajectories in quantum mechanics but there there may be angular momentum associated with electron in atom. It is a difficult problem but it can be proved that we can find the same eigenstates for complete system's Hamiltonian and for Hamiltonian describing only spin-orbit interaction [11]. Spin-orbit Hamiltonian in the matrix form is

$$\hat{H}_{SO} = \frac{\Omega}{3} \begin{pmatrix} 0 & -i & 0 & 0 & 0 & 1 \\ i & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & i & 0 \\ 0 & 0 & -1 & 0 & i & 0 \\ 0 & 0 & -i & -i & 0 & 0 \\ 1 & i & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (3.7)$$

where Ω is some number (a matrix element) and is not important here because its value will not be needed. One may ask in what basis we can write this Hamiltonian in that way. In

the $|J, m_j\rangle$ representation it is $\{|X \uparrow\rangle, |Y \uparrow\rangle, |Z \uparrow\rangle, |X \downarrow\rangle, |Y \downarrow\rangle, |Z \downarrow\rangle\}$ basis. The valence bands of certain materials consist of p - type atomic orbitals and for example $|X \uparrow\rangle$ denotes to p-orbital which posses probability distribution parallel to x -axis [9]. Its z -component of total angular momentum is positively oriented. Now, we just find Hamiltonian's eigenvectors. They are in the form [26]

$$|u_{lh\uparrow}\rangle = \left| \frac{3}{2}, \frac{1}{2} \right\rangle = \frac{1}{\sqrt{6}} |(X + iY) \downarrow\rangle - \frac{2}{\sqrt{3}} |Z \uparrow\rangle, \quad (3.8)$$

$$|u_{lh\downarrow}\rangle = \left| \frac{3}{2}, -\frac{1}{2} \right\rangle = -\frac{1}{\sqrt{6}} |(X - iY) \uparrow\rangle - \frac{2}{\sqrt{3}} |Z \downarrow\rangle, \quad (3.9)$$

$$|u_{hh\uparrow}\rangle = \left| \frac{3}{2}, \frac{3}{2} \right\rangle = \frac{1}{\sqrt{2}} |(X + iY) \uparrow\rangle, \quad (3.10)$$

$$|u_{hh\downarrow}\rangle = \left| \frac{3}{2}, -\frac{3}{2} \right\rangle = \frac{1}{\sqrt{2}} |(X - iY) \downarrow\rangle. \quad (3.11)$$

Indexes 'lh' and 'hh' mean light hole and heavy hole respectively. There are two more eigenvectors describing so called split-off bands but they are not of our interest. However, we should mention that in certain optically pumped spin-VCSELs electrons are being excited from split-off band states into conduction band states [19]. It is generally known that holes are quasi-particles. Here, the amplitudes of light hole and heavy hole bands represents rather states of electrons after recombination with light or heavy holes. After diagonalization of spin-orbit Hamiltonian one may find out that its spectrum is degenerated. It means that for one single energy eigenvalue there is more eigenstates. Light and heavy hole bands have the same energy near the band gap in a bulk material. However, it is not the case of quantum wells. When the quantum well potential is included in the Hamiltonian the eigenstates will split. There is thus some energy difference between light and heavy hole bands. Another examples of such splitting of degenerate states are Zeeman or Stark effects.

Finally we have to write wave function's amplitudes in bra-ket formalism of conduction band electrons. They are

$$u_{e\uparrow} = |S \uparrow\rangle \quad u_{e\downarrow} = |S \downarrow\rangle. \quad (3.12)$$

They differ from each other only in the projection of its spins. The symbol 'S' was used because conduction band electronic states are s - type orbitals [9].

3.3.2 Selection rules

It is important to realize that not all transitions in atoms or semiconductors are allowed. As we can see in the Appendix A, transitions are calculated using certain matrix elements. If such element is equal to zero, it means that given transition is not allowed. By studying matrix elements we may find what are allowed changes of quantum numbers during some

microscopic process. We can formulate so called electric dipole approximation selection rules that are [12]

$$\Delta m_j = \pm 1. \quad (3.13)$$

If we apply the selection rules to the possible quantum - mechanical states in a semiconductor quantum well we will see that only the following transitions are allowed

$$e \uparrow \rightarrow hh \uparrow, \quad e \uparrow \rightarrow lh \downarrow, \quad e \downarrow \rightarrow hh \downarrow, \quad e \downarrow \rightarrow lh \downarrow. \quad (3.14)$$

Another very important issue is the conservation of angular momentum. When a given transition occurs the particle may be created to compensate changes of quantum numbers. In this case it is photon with projection of total angular momentum $+1\hbar$ or $-1\hbar$. The sign depends on the transition. Now, it is important to define the axis of projection. Let it be the direction of propagation of photons-approximately perpendicularly on VCSEL's layers. Since there is a connection between photon's electromagnetic polarization and its projection of angular momentum on direction of propagation, the photon with $m_j = +1 \hbar$ is right-circularly polarized and $m_j = -1 \hbar$ is left-circularly polarized.

3.3.3 Probabilities of optical transitions

In order to calculate the probabilities of allowed optical transitions we should use famous Fermi golden rule. Fermi golden rule can be derived using time-dependent perturbation theory which is presented at the end of Appendix A [12]. Harmonic perturbation must be considered to derive it. Probability of the transition from initial state to final state per unit of time is

$$R_{i \rightarrow f} = \frac{2\pi}{\hbar} |W_{fi}|^2 \delta(\omega - \omega_{fi}). \quad (3.15)$$

Generally, the density of states should be included there. However, in case of quantum well's energy spectrum it can be neglected [10]. Here, W_{fi} is equal to $\langle u_f | \hat{\eta} \cdot \hat{E}_0 | u_i \rangle$, where $\hat{\eta}$ is the well-known electric dipole operator and \hat{E}_0 is the operator of electric field intensity amplitude. Dirac delta function is there because of the conservation of energy on the larger time-scales. Let us assume that electromagnetic wave interacting with system has only x and y components of electric field intensity. Only calculation needed to evaluation of the probability is the calculation of the matrix element. We consider the recombination of electron with the light hole. In order to get the form of matrix element we need, we will prove that $|\langle u_f | \hat{x} | u_i \rangle|^2 = |\langle u_i | \hat{x} | u_f \rangle|^2$ for an arbitrary Hermitian operator \hat{x} .

$$|\langle u_f | \hat{x} | u_i \rangle|^2 = \langle u_f | \hat{x} | u_i \rangle \langle u_f | \hat{x} | u_i \rangle^* = \langle u_i | \hat{x} | u_f \rangle^* \langle u_i | \hat{x} | u_f \rangle = |\langle u_i | \hat{x} | u_f \rangle|^2. \quad (3.16)$$

If electric field intensity of electromagnetic field interacting with system has only x-and y-components, we obtain

$$\langle u_{e\uparrow} | \hat{\eta} \cdot \hat{E}_0 | u_{lh\downarrow} \rangle = -\frac{1}{\sqrt{6}} \langle S \uparrow | \hat{\eta}_x \hat{E}_{0x} | X \uparrow \rangle + \frac{i}{\sqrt{6}} \langle S \uparrow | \hat{\eta}_y \hat{E}_{0y} | Y \uparrow \rangle. \quad (3.17)$$

Using results of more complex treatise on the topic [9] which is based on the spatial symmetry of p-like orbitals we can write that $\langle S \uparrow | \hat{\eta}_x \hat{E}_{0x} | X \uparrow \rangle = \langle S \uparrow | \hat{\eta}_y \hat{E}_{0y} | Y \uparrow \rangle = M$ ('M' as a matrix element). We have

$$\langle u_{e\uparrow} | \hat{\eta} \cdot \hat{E}_0 | u_{lh\downarrow} \rangle = -\frac{1}{\sqrt{6}}M + \frac{i}{\sqrt{6}}M \quad (3.18)$$

\Downarrow

$$\left| \langle u_{e\uparrow} | \hat{\eta} \cdot \hat{E}_0 | u_{lh\downarrow} \rangle \right|^2 = \frac{1}{3} |M|^2. \quad (3.19)$$

Inserting this result into Fermi golden rule we obtain

$$R_{e\uparrow \rightarrow lh\downarrow} = \frac{2\pi}{3\hbar} |M|^2. \quad (3.20)$$

This is the relative probability per unit of time of $e \uparrow \rightarrow lh \downarrow$ transition when system interacts with electromagnetic radiation. The same calculation can be performed in case of $e \uparrow \rightarrow hh \uparrow$, where we get

$$R_{e\uparrow \rightarrow hh\uparrow} = \frac{2\pi}{\hbar} |M|^2. \quad (3.21)$$

Thus, we obtained relatively well-known result, that heavy-hole transitions are three-times more probable than light-hole transitions [14]. Knowing this, there is the possibility of the polarization control of emitted light in case of spin-VCSELs. This will be discussed in the next section.

3.4 Polarization properties of spin-polarized VCSELs

We will analyze dynamical polarization properties of spin-VCSELs in this section. Spin-flip model and its solutions will be presented.

3.4.1 Spin - flip model

In the Chapter 2 we presented the derivation of Maxwell-Bloch equations using idealized two-level system. In case of much more complicated band structure of semiconductors in the presence of quantum well, the derivation is relatively difficult and time-consuming. Thus, we will not present it. The density matrix formalism should be used too [4]. In such derivation only heavy hole transitions are taking into account. It can be done because lasing modes that are generating by light hole transitions do not have to fulfill resonance conditions of cavity for example. This four-level approximation leads to the set of six coupled differential equations describing complex dipole moment densities of circularly polarized modes, two population inversions and complex electric field amplitudes. Since the dipole moment polarization relaxation rates are larger than those of other quantities, we can adiabatically

eliminate dipole polarizations [20]. We obtain following set of differential equations [19].

$$\frac{dN}{dt} = \gamma[\Lambda - (1 + |\mathbf{A}_+|^2 + |\mathbf{A}_-|^2)N - (|\mathbf{A}_+|^2 - |\mathbf{A}_-|^2)n], \quad (3.22)$$

$$\frac{dn}{dt} = \gamma P \Lambda - \gamma_s n - \gamma[(|\mathbf{A}_+|^2 + |\mathbf{A}_-|^2)n + (|\mathbf{A}_+|^2 - |\mathbf{A}_-|^2)N], \quad (3.23)$$

$$\frac{d\mathbf{A}_+}{dt} = \kappa(1 + i\alpha)(N + n)\mathbf{A}_+ - \kappa\mathbf{A}_+, \quad (3.24)$$

$$\frac{d\mathbf{A}_-}{dt} = \kappa(1 + i\alpha)(N - n)\mathbf{A}_- - \kappa\mathbf{A}_-. \quad (3.25)$$

Let us shortly discuss certain issues of development of these equations and then the meaning of each term. Originally, SFM (spin-flip model) was developed by San Miguel et al [20]. They used the model in order to analyze stability of different polarization modes in conventional VCSELs. At the time, they did not consider spin-polarized pumping. Their analysis was extended by Martin-Regalado et al[21]. It should be noted that they assumed the existence of anisotropies in real VCSEL structures which are important. Here, the anisotropies are not included.

Now, we want to explain meaning of each term. Let us consider population variables first. N and n are defined as

$$N = \frac{(e \uparrow + e \downarrow) - (hh \uparrow + hh \downarrow)}{2}, \quad n = \frac{(e \downarrow - hh \downarrow) - (e \uparrow - hh \uparrow)}{2}. \quad (3.26)$$

We used notation of electron and hole bands from previous section. However, for example $e \uparrow$ denote the spin-up electron concentration normalized to its threshold value [19]. The sense of populations chosen this way is not obvious at the first sight. Let us re-write $N + n$ and $N - n$ in terms of electron and hole bands.

$$N + n = e \downarrow - hh \downarrow, \quad N - n = e \uparrow - hh \uparrow. \quad (3.27)$$

If we recalled general rules for construction of such simplified Maxwell-Bloch equations or rate equations, we would see that $N + n$ should be always placed in terms describing stimulated emission of right-circularly polarized photon and vice-versa. It can be easily checked. To be sure, \mathbf{A}_+ , \mathbf{A}_- are complex slowly varying amplitudes of right- and left- circularly polarized light respectively. γ is decay rate of populations. κ is decay rate of field in the cavity and depends on its geometry. γ_s is spin relaxation rate. It is phenomenological parameter which represents numerous mechanisms of spin relaxation and can be measured. Γ stands for normalized pumping. α is the linewidth enhancement factor or sometimes called Henry's coefficient [21]. It represents coupling between amplitude and phase which arises from the fact that the refractive index of gain medium depends on carrier concentration. The last quantity P is the pumping polarization. We consider optical pumping and spin-VCSELs can be pumped by light that is composed of the mixture of right-and left-circularly polarized photons. If pumping is not polarized P is equal to zero. On the other side, if pumping is perfectly polarized P is equal to one. Sometimes the quantity is called polarization ellipticity.

It may model electrical pumping as well [7]. This term was not included in the original SFM developed by San Miguel et al.

Before we solve set of SFM equations, we want to note that the spontaneous emission was not included again. It can be done if the spontaneous emission has only slight effect on lasing process. However, the spontaneous emission is responsible for initiation of stimulated emission. This fact is not included in equations.

3.4.2 Solutions of SFM

SFM is set of coupled nonlinear differential equations, which is very difficult to solve without use of a computer. We decided to solve the equations with parameters that were measured and calculated recently. To be more precise, the calculation is based on parameters that can be found in paper written by Frougier et al. [7]. We should note, and it is very important, that studied laser had in this case VECSEL geometry. It means that it has only lower Bragg mirror and external output coupler. Then, a resonant cavity is more Fabry-Pérot-like, which simplify for example calculation of τ_{ph} , but this will be discussed later. Their structure consisted of DBR with 27.5 periods of AlAs/GaAs on GaAs substrate. The active region was formed by twelve $In_{0.22}Ga_{0.78}As/GaAs_{0.95}P_{0.05}$ quantum wells. In addition to this, there was MgO/Co/Pt spin-injector on the top of 1/2-VCSEL, how such structure is sometimes called. External cavity's optical element had reflectivity coefficient equal to 0.995.

Entire structure was optically pumped. Reported parameters of our interest are $\tau = \frac{1}{\gamma} = 1$ ns, $\tau_{ph} = \frac{1}{2\kappa} = 180$ ns, $\tau_s = \frac{1}{\gamma_s} = 60$ ps [7]. Henry's coefficient was chosen to be equal to 3.5. There is the experimental evidence that such devices has class A laser behavior which can be seen even from known lifetimes. Because of this we can adiabatically eliminate population variables. After doing so we have only differential equations describing \mathbf{A}_+ and \mathbf{A}_- with

$$N + n = \frac{\Lambda}{1 + I_+ + I_-} + \left[\frac{P(1 + 2I_-) - (I_+ - I_-) + \frac{(I_+ - I_-)}{(1 + I_+ + I_-)}}{\frac{\gamma_s}{\gamma}(1 + I_+ + I_-) + (1 + I_+ + I_-)(I_+ + I_-) - (I_+ - I_-)^2} \right] \Lambda, \quad (3.28)$$

$$N - n = \frac{\Lambda}{1 + I_+ + I_-} - \left[\frac{P(1 + 2I_+) - (I_+ - I_-) - \frac{(I_+ - I_-)}{(1 + I_+ + I_-)}}{\frac{\gamma_s}{\gamma}(1 + I_+ + I_-) + (1 + I_+ + I_-)(I_+ + I_-) - (I_+ - I_-)^2} \right] \Lambda, \quad (3.29)$$

where $I_{\pm} = |\mathbf{A}_{\pm}|^2$. We chose to calculate time-evolution of normalized intensities of two orthogonal polarizations. The calculation is presented in Figure 3.6. First of all, laser's behavior may be characterized as class A laser. We tried to demonstrate polarization control dependent on polarization ellipticity. It is not easy to find useful values for example of pumping rate because very often solution lost its stability.

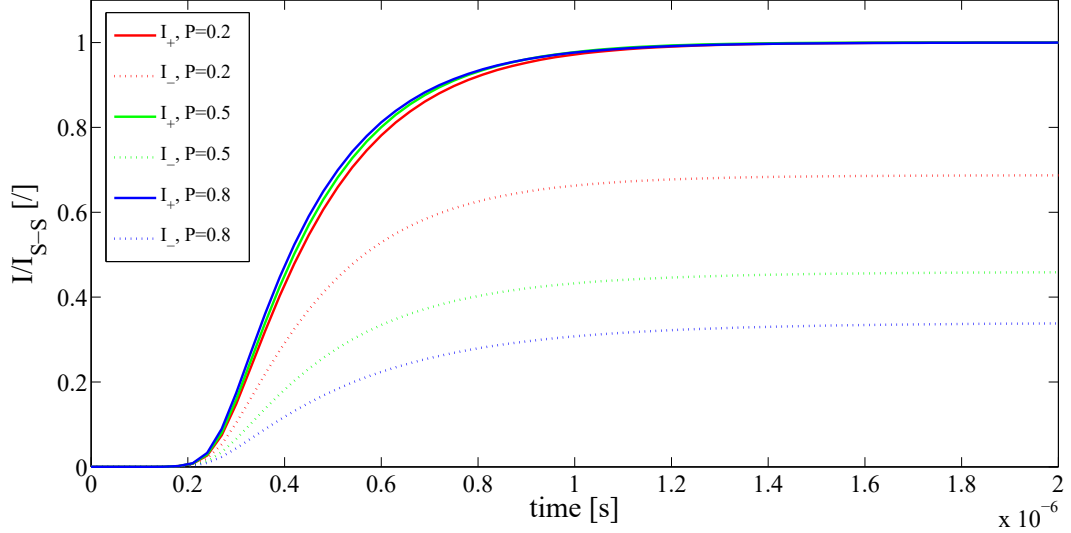


Figure 3.6: *The comparison of dynamical behavior of spin-VECSEL for different pump ellipticities. I_{S-S} is the intensity in steady-state. Normalization was performed with respect to stronger mode.*

Furthermore, we see in Figure 3.6 that with increasing pump ellipticity we observe that difference between orthogonal modes intensities are getting larger. If we take $P = 0$, both modes will have exactly the same solution because they will be pumped using non-polarized pump. However, if we had $P = 1$, both orthogonal modes would oscillate simultaneously, which is caused by the existence of spin-relaxation mechanisms. Assume that we pump the laser using perfectly right-circularly polarized light. In this case the population inversion would be established only on spin-down channel because without spin-relaxation mechanisms spin-up population would de-excite. However, spin-relaxation mechanisms are pushing the system into equilibrium and thus there is always the amount of spin-down electrons converted to spin-up per second.

Spin-flip model was also developed to describe so called polarization switching [21]. Suppose that laser is pumped with constant rate and emits light mode of certain polarization. If the pumping power is increased, the polarization of emitted light may switch to different mode. Such behavior was observed during numerical simulations. However, we are not sure if it was not just computational or interpretation mistake.

3.4.3 Anisotropies in V(E)CSEL structures

As we noted we did not included optical anisotropies in calculations. We should shortly discuss their meaning for lasing process. The presence of optical anisotropies in V(E)CSEL structures causes preference for two orthogonal linearly polarized modes [20, 21, 7]. We can pump spin-V(E)CSEL in order to obtain approximately circularly polarized emitted light but the polarization state of emitted light is changed by anisotropies. In practice, it could be for

example linear birefringence [21]. It means that the refractive index depends on polarization state of light passing through material. The anisotropies form mainly at interfaces between III-IV semiconductor layers due to T_d and C_{2V} symmetry breaking[25] or as a result of surface strain [19]. There are at least two more kinds of anisotropies. It is linear gain dichroism, which causes that two orthogonal linearly polarized modes has different gain-loss ratio. The second anisotropy is the magneto-optical anisotropy created by the magnetization of spin-injector. Anisotropies lead for example to different mode frequencies (frequency splitting) [7].

3.5 Mode competition

It is natural to expect coexistence of two laser modes in case of spin - lasers. Since spin-lasers are thought to be class A lasers, the population inversions may be neglected and it is possible to describe dynamics of spin-lasers using rate equations for intensities. Willis E. Lamb developed such model to describe multimode lasers in which he included terms describing how modes influence each other [4]. He formulated following nonlinear coupled differential equations of the first order

$$\frac{dI_+}{dt} = (G_+ - \beta_+ I_+ - \theta_{\pm} I_-) I_+, \quad (3.30)$$

$$\frac{dI_-}{dt} = (G_- - \beta_- I_- - \theta_{\mp} I_+) I_-, \quad (3.31)$$

where G_+ , G_- are non-saturated gain coefficients of right-circularly and left-circularly polarized modes respectively. Non-saturated gain means that gain is not lowered by high intensity of light in cavity. We may understand it as an effect of pumping. On the other hand, β_+ , β_- are self-saturation coefficients. They represent the effect of light intensity on gain of the same polarization mode. Finally, θ_{\pm} , θ_{\mp} are the cross-saturation coefficients which represent the influence of orthogonal polarizations on each other. Let us now define Lamb coupling coefficient as

$$C = \frac{\theta_{\pm} \theta_{\mp}}{\beta_+ \beta_-}. \quad (3.32)$$

It can be seen at the first sight that in case of $\theta_{\pm} = \theta_{\mp} = 0$ modes are not coupled and the set of equations is easy to solve. In order to make the analysis simpler, we take $\beta_+ = \beta_- = \beta$ and $\theta_{\pm} = \theta_{\mp} = \theta$. We know that there will be imbalance in gain when there is established assymetry in spin-up and spin-down populations. This can be described by introducing circular gain dichroism ΔG . Let us assume that preferred polarization will be right circular polarization:

$$G_+ = G + \frac{\Delta G}{2}, \quad G_- = G - \frac{\Delta G}{2}. \quad (3.33)$$

Since we do not know exact values of saturation coefficients, we will look for the steady - state solution. We get

$$I_+ = \frac{G(1 - \sqrt{C}) + \frac{\Delta G}{2G}(1 + \sqrt{C})}{\beta(1 - C)}, \quad (3.34)$$

$$I_- = \frac{G}{\beta} \frac{(1 - \sqrt{C}) - \frac{\Delta G}{2G}(1 + \sqrt{C})}{1 - C}. \quad (3.35)$$

The solution for different values of Lamb coupling constant can be seen in Figure 3.7. For $C = 0$ two modes are independent. As the Lamb coupling coefficient increases dominant mode becomes even more powerful. We see that curves in Figure 3.7 are not smooth at certain points. It has two reasons. The first is that the intensity cannot be negative. The second reason is, that if we eliminate weaker mode, the dominant one must be described by equations with $C = 0$.

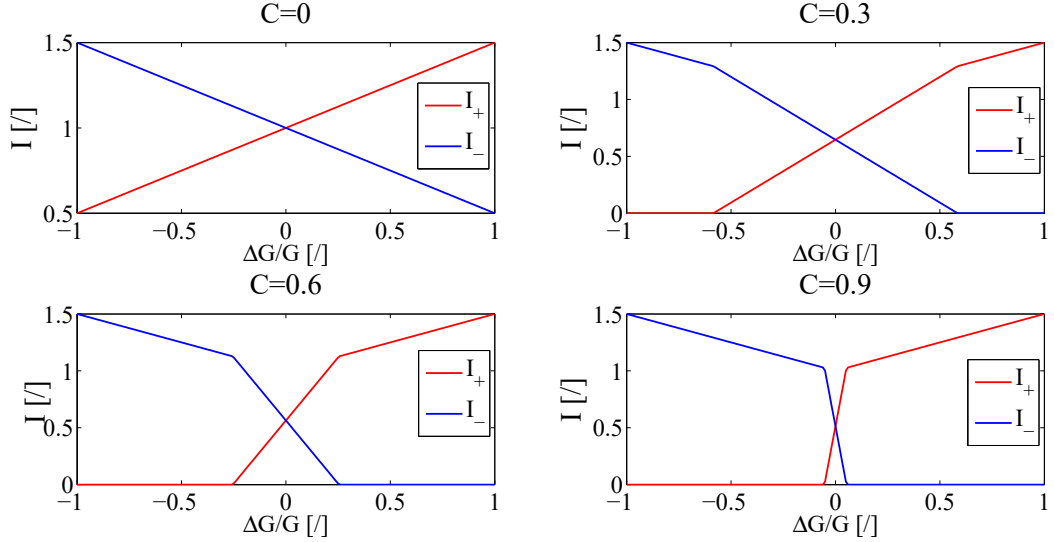


Figure 3.7: *Steady-state intensity as a function of normalized gain dichroism for different values of Lamb coupling constant.*

Frougier et al. reported that for their VECSEL structure $C \cong 0.9$. As we can see in Figure 3.7 there is very small interval of gain dichroism in which modes can oscillate simultaneously in case of such large coupling constant. The most interesting aspect is that even with that small values of dichroism we can achieve nearly 100% right- or left-circularly polarized light. When we take $\Delta G = 0$, steady-state intensities of both modes are equal to each other. It could be expected because in such state both modes are amplified equally and this state is not dependent on a value of coupling constant. On the other hand, if we have $C = 0$ and at the same time $\Delta G \neq 0$, intensities depend only on gain dichroism. We see that two modes can coexist if $\frac{\Delta G}{G} \in (-1, 1)$. If we were able to obtain $\frac{\Delta G}{G} = 1$ it would mean that $\Delta G = G$ and thus only one mode can oscillate. For $C \cong 1$ solution diverges and infinitesimally small gain dichroism causes the elimination of weaker mode.

Chapter 4

Application of SFM to model VCSEL structures

As we noted many times, dynamics of laser is given by values of time parameters that are specific for a given gain medium and for a resonant cavity. For example population inversion lifetimes can be modified by changing temperature but we assume that the temperature is constant here. Of course the pumping rate has an effect on dynamical properties of the laser [21]. However, these effects have only quantitative character if we neglect issues as polarization switching caused by changes in pumping. On the other hand, we are able to modify laser behavior by changing parameters of optical cavity. In this chapter we will apply more general method of photon lifetimes calculations. Calculated parameters will be used during solution of SFM equations.

4.1 More general method of τ_{ph} calculation

In case of a simple Fabry-Pérot resonant cavity we used the following algorithm in order to calculate resonator losses. We let photons to make round-trip in a resonator. Then we evaluated total energy losses during round-trip. Next, the time duration of one round-trip was calculated and finally we obtained the photon lifetime. VCSELs have complicated multilayered reflectors. Thus, as far as we know it is not possible to use round-trip approximation. To be more precise, it is possible but we do not know if it would give approximately correct answers. It would be complicated even with just for example five layers in each of DBR. However, it is possible to evaluate losses per unit of time from spectral response of cavity. We should note that at least two approximations must be used in this case. The first is that spectral response of passive resonator is not exactly the same as of the active resonator (with gain medium) [1]. The second approximation is that we neglect the influence of spin-injector. In practice, spin-injector could be located in region where electromagnetic waves interfere destructively in order to minimize its effect.

Let us assume that decay of the electric field intensity amplitude E_0 inside the passive

resonator can be described by

$$\frac{dE_0}{dt} = -\kappa E_0, \quad (4.1)$$

where $\kappa = \frac{1}{2\tau_{ph}} = \frac{1}{\tau_E}$ is decay rate of field inside cavity. It means that electric field intensity at fixed point inside resonator will behave as

$$E(t) = E_0(0) \exp\left[i2\pi\nu_0 t - \frac{t}{\tau_E}\right]. \quad (4.2)$$

Let us now calculate Fourier transform

$$F(\nu) = E_0(0) \int_0^\infty \exp\left[i2\pi\nu_0 t - \frac{t}{\tau_E}\right] e^{-i2\pi\nu t} dt = \frac{E_0(0)}{\frac{1}{\tau_E} + i2\pi(\nu - \nu_0)}. \quad (4.3)$$

Next, we want to know what the intensity is as a function of ν . It is

$$I(\nu) = \frac{I_0}{\left(\frac{1}{\tau_E}\right)^2 + 4\pi^2(\nu - \nu_0)^2}. \quad (4.4)$$

This is Lorentzian distribution with peak at ν_0 and it turns out that there is a connection between its **F**ull **W**idth at **H**alf **M**aximum ($\Delta\nu$) and field decay rate [1]. We can easily find after simple calculation that

$$\tau_E = \frac{1}{\pi\Delta\nu}. \quad (4.5)$$

Since we work primary with wavelengths we can rewrite it by using

$$\frac{d\nu}{d\lambda} = -\frac{c}{\lambda^2} \quad \Rightarrow \quad \Delta\lambda = \frac{\lambda^2}{c} \Delta\nu, \quad (4.6)$$

where it is possible to take $\lambda = \lambda_0$. Finally, we can write down that

$$\tau_{ph} = \frac{1}{2\pi} \frac{\lambda_0^2}{c\Delta\lambda}. \quad (4.7)$$

This method is powerful in our case because we are able to calculate precisely $\Delta\lambda$ using matrix formalism presented in Appendix B. However, spectral response of resonant cavity has to be approximately Lorentzian. We see that $\tau_{ph} \propto \frac{1}{\Delta\lambda}$. It is qualitatively a correct result, because we may expect that the smaller energy losses of resonator are the sharper will be its spectral response.

4.2 τ_{ph} of VCSEL's resonant cavity

In this section, we want to demonstrate how exactly τ_{ph} relates to the number of periods of VCSEL's reflectors. We chose to model VCSEL as a GaAs layer between two AlAs/GaAs Bragg reflectors. In practice, it would not be a good geometry, because quantum well region and DBR would be nearly indistinguishable. We should note that the layer representing quantum well region has different thickness than GaAs layers in DBR. Lower DBR has always more periods than the upper one in our case. For example 10-5 means that lower DBR has

10 periods and upper one has 5 periods of AlAs/GaAs. We present the calculation of 15-10 configuration spectral response below. The calculation is based on formalism presented in Appendix B. The matrix of entire structure was constructed and then we calculated the intensity of transmitted light for set of wavelengths from certain interval. We considered only normal incidence of light.

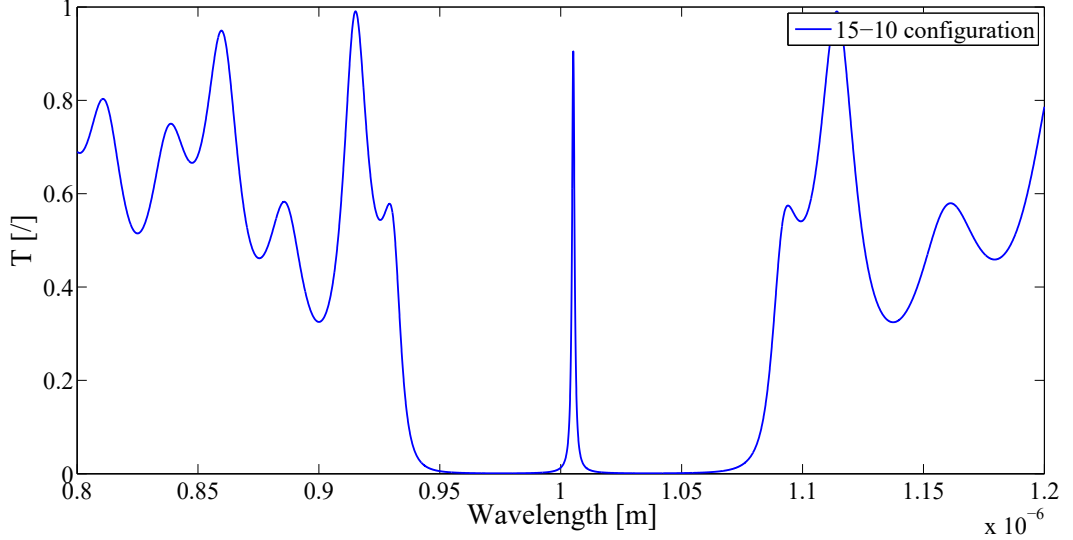


Figure 4.1: *Calculated spectral response of 15-10 configuration with sharp peak at the center. T is a ratio of transmitted light intensity to intensity of incident light.*

During the calculation of τ_{ph} we contract the wavelength interval in order to consider only central peak. Resonance peaks of different configurations are presented in Figure 4.2.

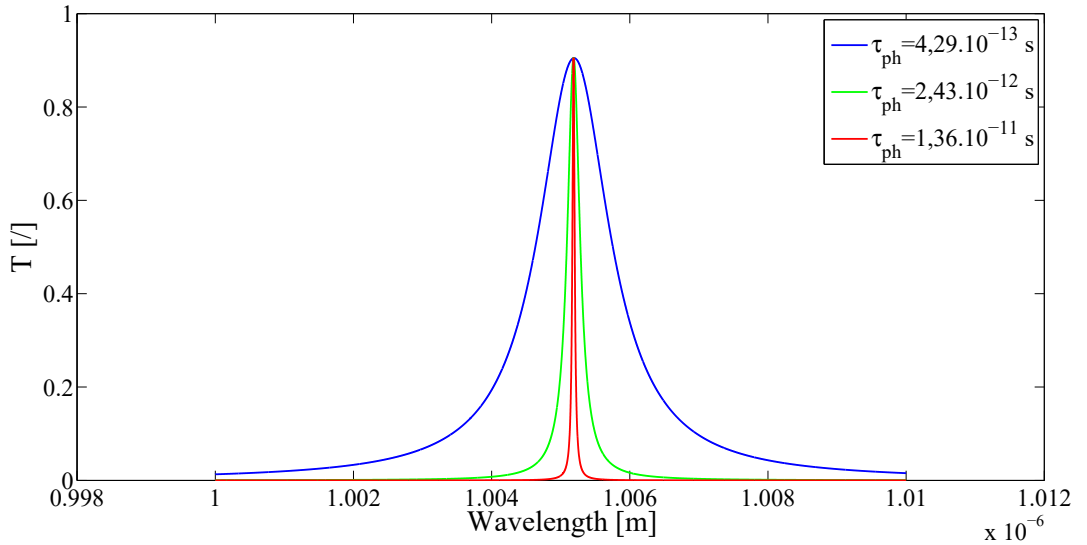


Figure 4.2: *Calculated spectral response and τ_{ph} of different VCSEL resonant cavities near resonant wavelength.*

The first (blue) curve in Figure 4.2 was calculated for 15-10 configuration. τ_{ph} is in order

of 10^{-13} s. Note that VECSEL structure reported by Frougier et al. was characterized by $\tau_{ph} = 180$ ns. Laser with that small photon lifetime would not behave as class A laser. Real DBR in VCSELs contain more periods, however. For this reason we performed the same calculation for 20-15 configuration which is represented by green curve. As we expected $\Delta\lambda$ is much smaller and thus τ_{ph} is larger and very close to values reported in literature [21]. The last calculation was performed for 25-20 configuration (red color). As far as we know, even these parameters are not specific for class A. This will manifest itself in the next section where we will solve SFM equations with parameters calculated here.

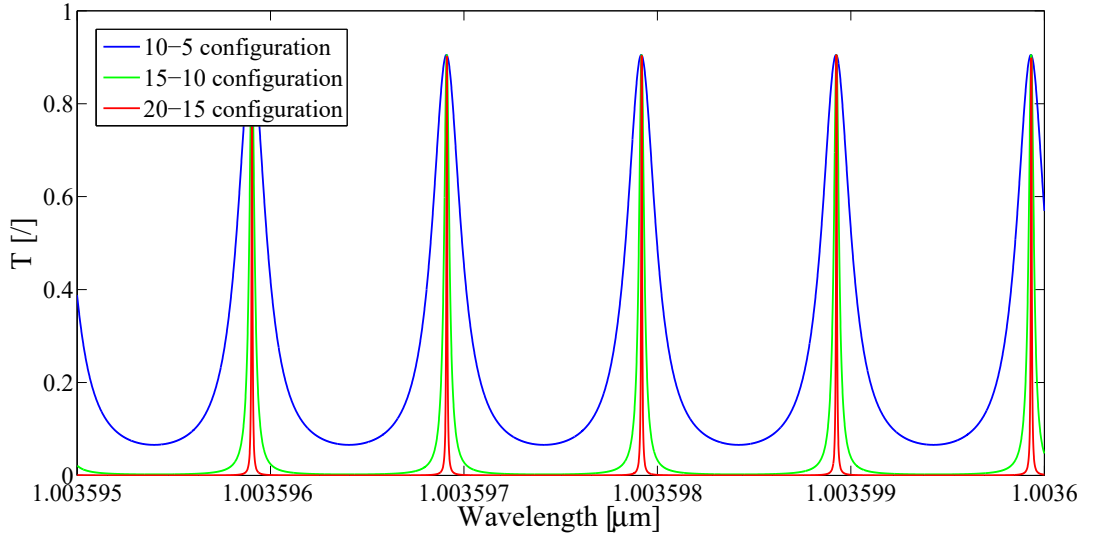


Figure 4.3: *Calculated spectral response of VECSEL resonant cavity in a range of wavelengths from 1.003595 μm to 1.0036 μm . Air gap between two DBR is 0.5 m.*

If the length of cavity increases, as in case of VECSELs, a resonant cavity will begin to behave like Fabry-Pérot cavity. It can be seen in Figure 4.3 that the spectral response has typical Fabry-Pérot characteristics which is different for VCSEL resonator, where spectral response does not possess such symmetry. In Figure 4.2 we chose to show only one peak that formed approximately at the center of DBR's band gap. In case of VECSEL it is possible to calculate photon lifetimes using the round-trip approximation. Additionally we may observe that even with small number of periods of used DBR $\Delta\lambda$ is much smaller. 20-15 VECSEL configuration gives $\tau_{ph} = 94$ ns and consequently class A laser behavior.

4.3 Modeling of spin-VCSEL's dynamics

In the last section we want to use some of the results obtained in the previous section. We will analyze behavior of spin-VCSEL using again spin-flip model. We should remember that modeled structures are idealized. However, based on analysis of photon lifetimes in VCSEL structures in the previous section, we can say that it is not possible to use spin-flip model

with adiabatically eliminated populations. It is not possible, because τ_{ph} are by orders of magnitude smaller than τ . We will not solve SFM equations for 15-10 configuration because calculated photon lifetime is very small and it could be beyond the interval of SFM validity. Method we consider to be more precise is currently under development and we will discuss it at the end of thesis. On the other hand, we will perform calculations for 20-15 configuration. We will use the same spin relaxation and population relaxation parameters as previously in order to simplify calculations.

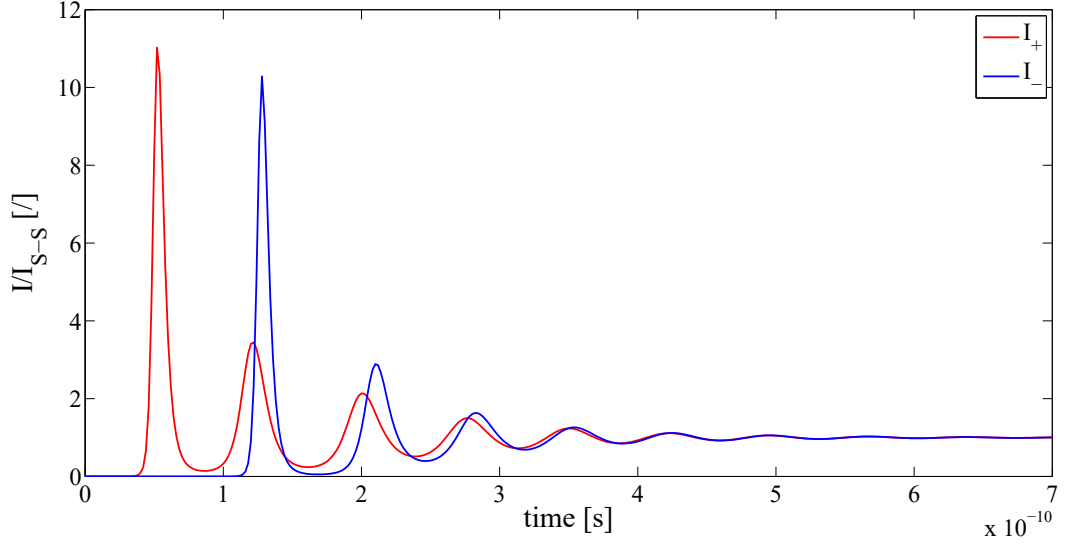


Figure 4.4: *Spin-flip model prediction of spin-VCSEL dynamics for $P = 0$ and $\tau_{ph} = 2.43$ ps. I_{S-S} is intensity of light in steady-state*

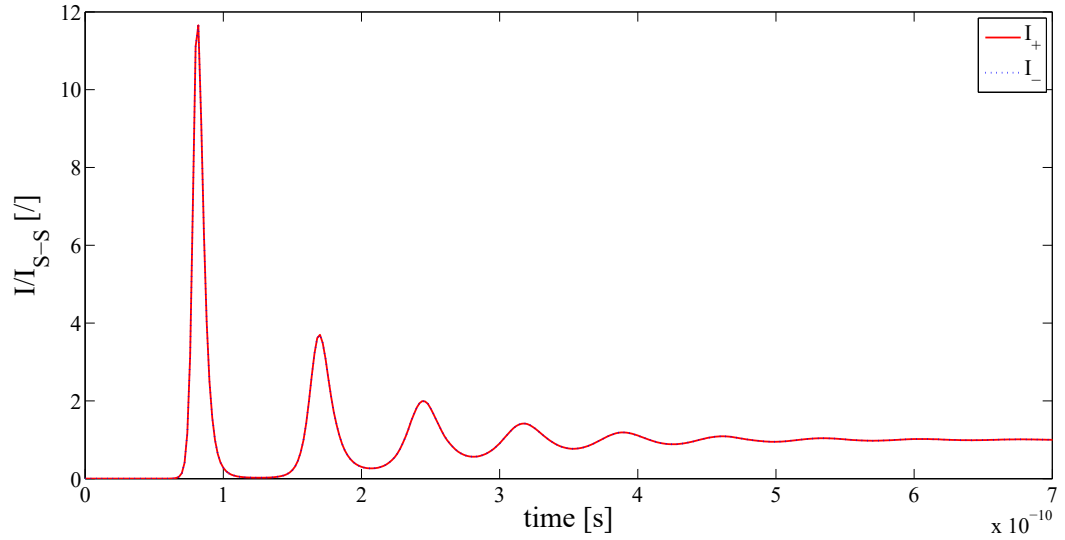


Figure 4.5: *Spin-flip model prediction of spin-VCSEL dynamics for $P = 0$, $\tau_{ph} = 2.43$ ps, $n(0) = 0$ and $N(0) = 1$.*

Let us first consider the case with non-polarized pumping (see Figure 4.4). As we ex-

pected, the steady-state solutions of right- and left-circularly polarized modes are identical. On the other side, it was not obvious that their evolution before reaching the steady-state is not same. It turns out that it is an effect of initial conditions. We should begin the calculations in non-polarized state. It can be done by taking $n(0) = 0$ as can be seen from its definition. After doing so we really obtain exactly the same solution for both polarizations (see Figure 4.5). We assume that it is a good approximation that spins of carriers are non-polarized at room temperature. At very low temperatures the situation can be different. The interpretation is clear. In case where we begin the calculation with $n(0) \neq 0$ (here, it was $n = 1$) left-circularly polarized mode will be amplified with a different rate compared to right-circularly polarized mode because there are different population inversions on two channels with opposite spin. However, laser is pumped with $P = 0$ and additionally there are spin relaxation mechanisms described by τ_s that together are pushing two polarization modes into an equilibrium.

In Figure 4.6 we see the time-evolution of normalized intensities of two orthogonal polarization modes for $P = 0.3$. The normalization was performed with respect to steady-state value of preferred mode intensity. In comparison with modeled VECSEL in the previous chapter there are at least three differences. The first is a typical class B laser behavior which is given by proportions of lifetimes. Let us recall that at the end of the second chapter we compared different laser classes and class B laser reached steady-state later than class A laser. It is caused by the fact that values of lifetimes are much smaller than those in the second chapter. As far as we know, faster dynamics is one of the promise of spin-VCSELs [19]. However, it is questionable if we are able to approximately describe such fast processes using spin-flip model. In such case dipole moment density relaxation must be by orders of magnitude faster than decay of electric field.

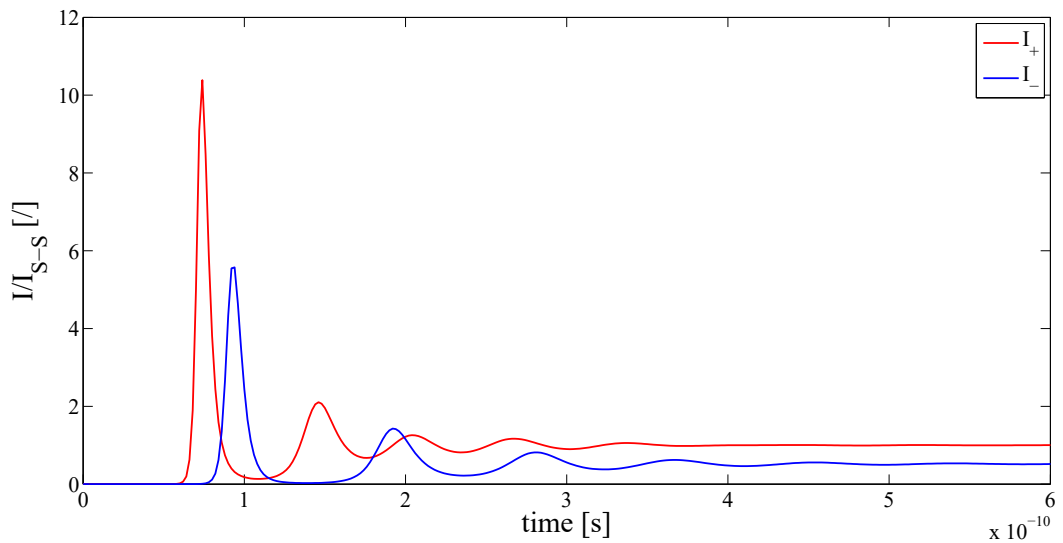


Figure 4.6: *Spin-flip model prediction of spin-VCSEL dynamics for $P = 0.3$ and $\tau_{ph} = 2.43$ ps.*

From a polarization control perspective spin-VCSELs seem to have a better performance than modeled VECSEL. Note that modeled VECSEL was pumped optically. On the other side spin-VCSELs are mostly pumped electrically. However, spin-flip model equations are general from this point of view and electrical pumping can be modeled as well as optical one. In Figure 4.7 and Figure 4.8 we demonstrate that with increasing pump ellipticity the intensity of weaker mode goes to zero. It can be seen that preferred polarization begin to oscillate earlier and this difference is proportional to value of pump ellipticity.

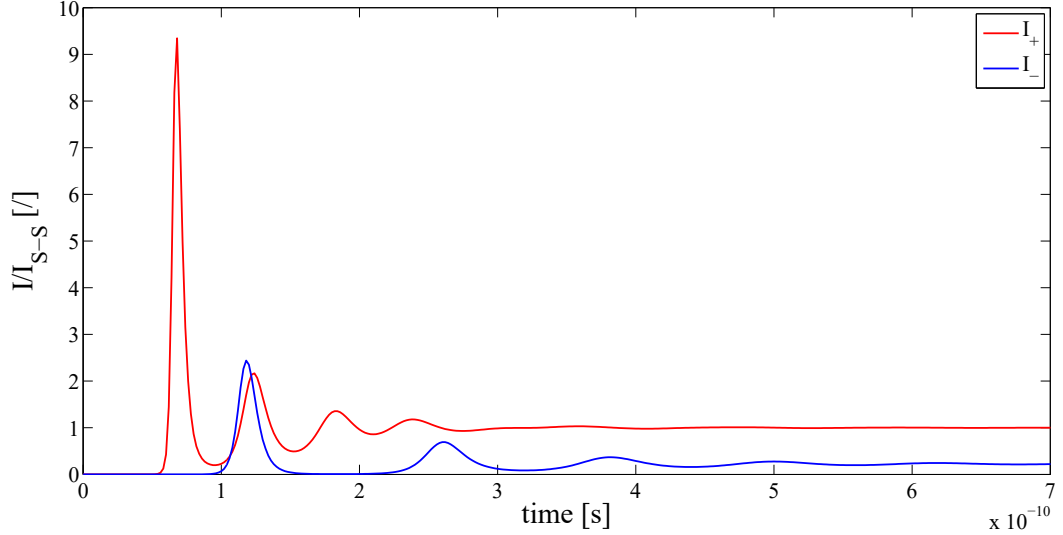


Figure 4.7: *Spin-flip model prediction of spin-VCSEL dynamics for $P = 0.6$ and $\tau_{ph} = 2.43$ ps.*

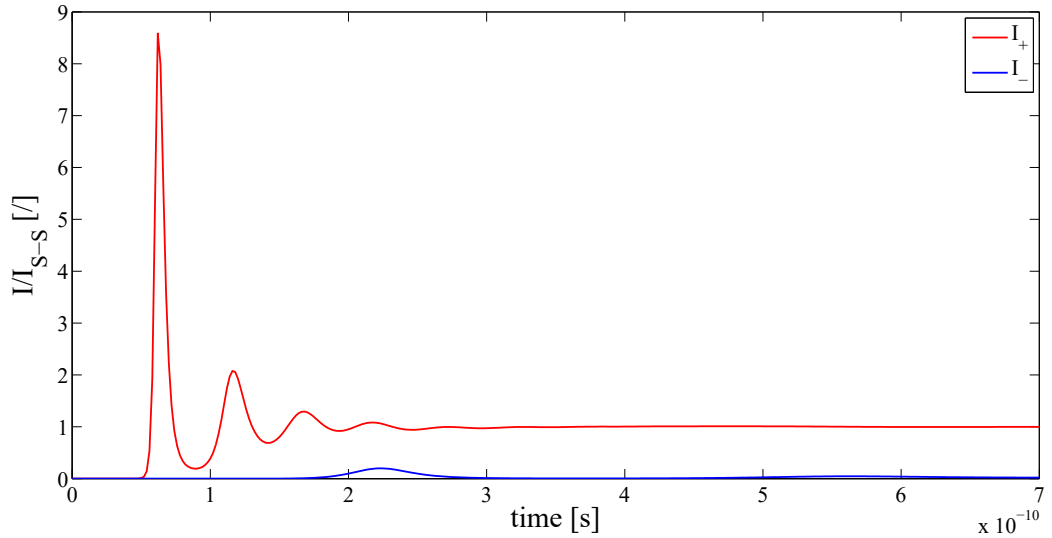


Figure 4.8: *Spin-flip model prediction of spin-VCSEL dynamics for $P = 0.9$ and $\tau_{ph} = 2.43$ ps.*

As it was indicated, we would obtain much better description of spin-VCSEL dynamics if

we used rigorous Maxwell-Bloch equations. On the other side, this would be computationally more challenging and very often it is difficult to find suitable parameters such as dipole moment or relaxation rate of atomic coherences (valence-conduction bands coherences in this case).

Chapter 5

Conclusions and perspectives

The goal of this bachelor thesis was modeling of dynamical properties of spin-polarized lasers. During the elaboration of thesis I had an occasion to study and understand basics of laser physics and physics of spin-polarized lasers. The main results of this bachelor thesis are:

- modeling of spectral response of multilayered V(E)CSEL's resonant cavities which enabled me to calculate photon lifetimes,
- numerical solution and analysis of SFM equations that describe dynamical properties of spin-polarized lasers,
- experimental and theoretical study of Bragg mirror used in V(E)CSEL structures using Mueller matrix ellipsometry.

In my future work, I would like

- to sophisticate and improve the model which was partially developed during elaboration of this thesis. The approach is more exact and is based on the combination of the Yeh's matrix formalism(for one active region [18]), Scattering matrix formalism(for multiple active region [27]) and the complete Maxwell-Bloch equations,
- to include local optical anisotropies such as interface and surface anisotropies and realistic multiple quantum well region to model dynamical properties of spin-V(E)CSEL laser structures.

Results of this work will be presented at NanoOstrava 2017 conference.

Appendices

Appendix A

The fundamentals of quantum mechanics

In the following appendix there are presented rather basic ideas and formal structure of quantum mechanics. Despite that, the chapter may include more advanced parts of quantum mechanics because they are needed for full understanding of thesis. For this reason, it can be seen as incomplete. However, it is not possible to make complete presentation of quantum mechanics here.

A.1 Postulates of quantum mechanics

In the beginning of the 20. century there was a need for a new physical theory (let us neglect issues with theory of relativity here). It was caused by the fact that the classical physics was unable to describe atomic structure of matter or some aspects of radiation. Numerous experiments were performed indicating that the classical physics was not complete description of nature. Based on experiments, people like Heisenberg, Schrödinger, Dirac and others developed the quantum mechanics [12]. The main ideas can be presented using so called postulates of quantum mechanics [13].

Let us begin with **”the wavefunction postulate”**. The electron is a typical object that must be treated quantum - mechanically. Instead of writing down its position and momentum as in a classical framework we describe quantum-mechanical system (such as the electron) using the wavefunction $\psi(\mathbf{r}, t)$. Sometimes it is called the probability amplitude because quantum mechanics provides only probabilistic description of nature. It contains all the informations about the electron. We will see later how we can extract them from the wavefunction. $\psi(\mathbf{r}, t)$ is generally the complex function. If we wanted to find the electron we would define the probability density[12]

$$\frac{dP}{dV} = \psi^*(\mathbf{r}, t)\psi(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2. \quad (\text{A.1})$$

We see that if we wanted to know what is probability of finding electron in certain space interval we would simply integrate the probability density over such interval. The wavefunction must be normalized so that the probability of finding the electron somewhere in space is equal to 1.

The next postulate is **"the operators postulate"**. We can associate linear Hermitian operator to each physical quantity that can be measured. In order to find possible values of a given quantity we should act on the wavefunction with the operator [13].

How exactly we can calculate possible values of certain quantity is described by **"the quantization postulate"**. When we perform the measurement on quantum-mechanical system all possible values we can obtain are given by spectrum of operator for a given quantity. The spectrum of operator can be found by solving eigenvalue problem [13]:

$$\hat{x}\phi_n = x_n\phi_n, \quad (\text{A.2})$$

where x_n is n-th eigenvalue and ϕ_n is n-th eigenfunction. Let us mention that system's wavefunction can be written as a superposition of eigenfunctions which will be slightly clearer later when we introduce bra-ket notation

$$\psi = \sum_n c_n \phi_n. \quad (\text{A.3})$$

When we are discussing the measurement we should mention **"the collapse of wavefunction postulate"**. If we measure x_n the system immediately collapses into state ϕ_n . The probability of measuring the x_n is given by

$$P_n = |c_n|^2. \quad (\text{A.4})$$

The last postulate is **"the Schrödinger equation postulate"**. It tells that time-evolution of system described by ψ is governed by the time-dependent Schrödinger equation [13, 12]

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \hat{H} \psi(\mathbf{r}, t), \quad (\text{A.5})$$

where \hat{H} is Hamiltonian-operator of energy. The set of postulates sometimes differs from book to book. However, we think it contains all important ideas of quantum mechanics.

A.2 Bra-ket notation

One of the founders of quantum mechanics, Paul Adriene Maurice Dirac, came with very elegant bra-ket notation. It is based on the idea that states of system can be represented as vectors in linear spaces. Then, we work with operators as with matrices which is natural because eigenvalue problem is typical procedure in case of matrices. Ket and bra-vectors

can be written respectively as [12]

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}, \quad \langle\psi| = (c_1^*, c_2^*, \dots, c_n^*). \quad (\text{A.6})$$

One may ask what is the basis of those vectors. It depends on physical situation but usually we work with energy eigenstates-eigenvectors of Hamiltonian. Let us now assume that $\{|\phi_n\rangle\} \Leftrightarrow \{|n\rangle\}$ will always be our basis. Such basis must be orthonormal. It means that relations $\langle n|n\rangle = 1$ and $\langle m|n\rangle = \delta_{mn}$ are fulfilled [12].

In the bra-ket notation scalar product is defined as

$$\langle\phi|\varphi\rangle = \sum_n \langle\phi|n\rangle \langle n|\varphi\rangle = \sum_n a_n^* b_n, \quad (\text{A.7})$$

where $a_n^* = \langle\phi|n\rangle$ and $b_n = \langle n|\varphi\rangle$. We can write it in the continuous basis as well:

$$\langle\phi|\varphi\rangle = \int \langle\phi|\mathbf{r}\rangle \langle\mathbf{r}|\varphi\rangle d\mathbf{r} = \int \phi^*(\mathbf{r})\varphi(\mathbf{r})d\mathbf{r}. \quad (\text{A.8})$$

The projection operator was used there and we will define it below. The scalar product is very important operation in quantum mechanics because $\langle\phi|\varphi\rangle$ is the projection of state $|\varphi\rangle$ onto state $|\phi\rangle$. In different words, it has a meaning of probability amplitude of process in which state $|\varphi\rangle$ will change to $|\phi\rangle$. It is important to note that the one of the advantages of bra-ket notation is that it does not matter what representation we work with. The wavefunction can be written in the position representation as

$$\psi(\mathbf{r}) = \langle\mathbf{r}|\psi\rangle. \quad (\text{A.9})$$

If we wanted to work with momenta we would just make projection of state vector onto momentum eigen-bra [12].

As it was indicated it is important to introduce the projection operator [12]

$$\hat{P} = \sum_n |n\rangle \langle n| \quad \text{or in case of continuous basis:} \quad \hat{P} = \int |\mathbf{r}\rangle \langle\mathbf{r}| d\mathbf{r}. \quad (\text{A.10})$$

In order to see what is this good for let us act with it on state vector ψ :

$$\hat{P}|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle = \sum_n c_n |n\rangle = |\psi\rangle. \quad (\text{A.11})$$

Recall that $\langle n|\psi\rangle$ is projection of state vector onto n-th eigenvector which is equal to c_n . Now it is clear why the state vector can be written as a superposition of eigenvectors in a given basis.

Let us now shortly discuss properties of operators. An arbitrary operator \hat{x} can be represented as a matrix in linear n-dimensional vector space:

$$\hat{x} = \begin{pmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nn} \end{pmatrix}. \quad (\text{A.12})$$

Very often we have to calculate the matrix element. Let us calculate for example x_{mn} [12]

$$x_{mn} = \langle m | \hat{x} | n \rangle. \quad (\text{A.13})$$

It can be easily checked performing calculations with vectors and matrix. The last aspect to mention is the calculation of the mean value of quantity x which is defined in the following way [12]:

$$\langle \hat{x} \rangle = \langle \psi | \hat{x} | \psi \rangle \quad (\text{A.14})$$

Finally, we will make a little repetition of mathematical ideas behind the quantum mechanics. We work only with energy eigenstates so we will limit our considerations to it. Additionally, we work mostly with systems of discrete spectrum. The state of system is then described by the state vector which time-evolution is governed by the Schrödinger equation. The state vector is a superposition of energy eigenvectors and when we perform the measurement on the system the system will collapse to one of its eigenstates. Mathematically, we just calculate the scalar product of a given eigenvector and the state vector which is equal to finding projection of the state vector onto given eigenvector [12].

A.3 The general solution of Schrödinger equation

In this section we will see how to obtain general solution of the Schrödinger equation. We assume that system's Hamiltonian is time-independent. In this case we can re-write the wavefunction as

$$\psi(\mathbf{r}, t) = \phi(\mathbf{r})\varphi(t). \quad (\text{A.15})$$

Let us insert this into time-dependent Schrödinger equation and re-arrange it so that we have

$$i\hbar \frac{1}{\varphi(t)} \frac{d\varphi(t)}{dt} = \frac{1}{\phi(\mathbf{r})} \hat{H} \phi(\mathbf{r}) = E \quad (\text{A.16})$$

\Downarrow

$$i\hbar \frac{1}{\varphi(t)} \frac{d\varphi(t)}{dt} = E, \quad \frac{1}{\phi(\mathbf{r})} \hat{H} \phi(\mathbf{r}) = E, \quad (\text{A.17})$$

where we added constant E . It can be done because both sides must be equal and the term with time-independent Hamiltonian indicates that its equal to energy. We obtained two

equations which we know how to solve. Take the time-dependent equation first. Its solution is

$$\varphi(t) = e^{-i\frac{E}{\hbar}t}. \quad (\text{A.18})$$

It represents harmonic oscillations. The second one is something we know-the eigenvalue problem. We obtain spectrum of possible energies:

$$\hat{H}\phi_n(\mathbf{r}) = E_n\phi_n(\mathbf{r}). \quad (\text{A.19})$$

The general solution of the time-independent part can be written as

$$\phi(\mathbf{r}) = \sum_n c_n \phi_n(\mathbf{r}). \quad (\text{A.20})$$

Additionally we can re-write $E \rightarrow E_n$ in time-dependent part because we know from stationary solution that E represents set of possible energies E_n . Finally we can write down the complete general solution:

$$\psi(\mathbf{r}, t) = \phi(\mathbf{r})\varphi(t) = \sum_n c_n \phi_n(\mathbf{r}) e^{-i\frac{E_n}{\hbar}t}. \quad (\text{A.21})$$

Since we work mostly with bra-ket notation let us re-write it knowing that $\langle \mathbf{r} | \psi(t) \rangle$ and $\langle \mathbf{r} | \phi_n \rangle$ [12]:

$$|\psi(t)\rangle = \sum_n c_n |\phi_n\rangle e^{-i\frac{E_n}{\hbar}t} = \sum_n c_n |n\rangle e^{-i\frac{E_n}{\hbar}t}. \quad (\text{A.22})$$

A.4 Time-dependent perturbation theory

In the previous section we presented general solution of system with time-independent Hamiltonian. It could be for example some idealized simple atom where the Hamiltonian represents the Coulomb interaction of electrons and nucleus. We can make the Hamiltonian time-dependent simply by placing such atom into oscillating electromagnetic field. The Hamiltonian then becomes

$$\hat{H}(t) = \hat{H}_0 + \hat{W}(t), \quad (\text{A.23})$$

where $\hat{W}(t)$ represents the perturbation. We know that the general solution of the Schrödinger equation with Hamiltonian \hat{H}_0 is

$$|\psi(t)\rangle = \sum_n c_n |n\rangle e^{-i\frac{E_n}{\hbar}t} = \sum_n c_n |n(t)\rangle. \quad (\text{A.24})$$

Let us assume that we want to find probability of measuring n -th state:

$$P_n = |\langle n | \psi(t) \rangle|^2 = \left| c_n e^{-i\frac{E_n}{\hbar}t} \right|^2 = |c_n|^2. \quad (\text{A.25})$$

The probability is time-independent. This is different in case of time-dependent Hamiltonian. Let us have a general solution

$$|\psi(t)\rangle = \sum_n c_n(t) |n(t)\rangle \quad \text{with} \quad |n(t)\rangle = |n\rangle e^{-i\frac{E_n}{\hbar}t}. \quad (\text{A.26})$$

Now, we have to write down the Schrödinger equation with assumed general solution:

$$i\hbar \sum_n \frac{d}{dt} [c_n(t) |n(t)\rangle] = [\hat{H}_0 + \hat{W}(t)] \sum_n c_n(t) |n(t)\rangle. \quad (\text{A.27})$$

After evaluating derivatives and taking into account that $\hat{H}_0 |n(t)\rangle = E_n |n(t)\rangle$ we get [12]

$$i\hbar \sum_n \frac{dc_n(t)}{dt} |n(t)\rangle + i\hbar \sum_n c_n(t) \frac{|n(t)\rangle}{dt} = \sum_n c_n(t) E_n |n(t)\rangle + \sum_n c_n(t) \hat{W}(t) |n(t)\rangle \quad (\text{A.28})$$

\Downarrow

$$i\hbar \sum_n \frac{dc_n(t)}{dt} |n(t)\rangle = \sum_n c_n(t) \hat{W}(t) |n(t)\rangle. \quad (\text{A.29})$$

At this point we will act on both sides of equation using m-th eigen-bra vector so the equation becomes

$$i\hbar \sum_n \frac{dc_n(t)}{dt} \langle m(t)|n(t)\rangle = i\hbar \sum_n \frac{dc_n(t)}{dt} \delta_{mn} = \sum_n c_n(t) \langle m(t)| \hat{W}(t) |n(t)\rangle. \quad (\text{A.30})$$

We perform summation over n so that we obtain

$$i\hbar \frac{dc_m(t)}{dt} = \sum_n c_n(t) \langle m| \hat{W}(t) |n\rangle e^{i\frac{\hbar}{\hbar}(E_n - E_m)t} = \sum_n c_n(t) W_{mn}(t) e^{i\omega_{mn}t}. \quad (\text{A.31})$$

It can be seen that it is set of differential equations. To make it clearer we can re-write it into matrix form because $W_{mn}(t)$ stands for the matrix elements.

$$\frac{d}{dt} \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} = \frac{1}{i\hbar} \begin{pmatrix} W_{11}(t) & \cdots & W_{1n}(t)e^{i\omega_{1n}t} \\ \vdots & \ddots & \vdots \\ W_{n1}(t)e^{i\omega_{n1}t} & \cdots & W_{nn}(t) \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}. \quad (\text{A.32})$$

Appendix B

Propagation of electromagnetic waves in a multilayer

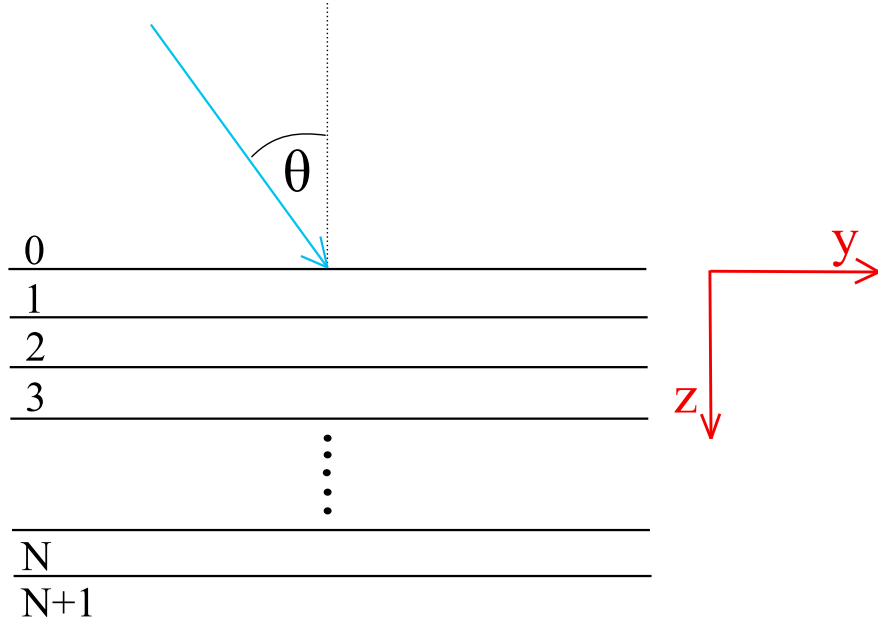


Figure B.1: .

Let us have a system that consists of N layers with coordinate system as in Figure B.1. Very often we need to calculate reflectivity coefficients or electric field distribution of such system. It is clear that it is highly impractical to use conventional methods such as construction of reflectivity coefficients using Fresnel's equations. We have to use more sophisticated and general framework-Yeh's matrix formalism [24, 3], which will be presented below. Note that each layer could be optically anisotropic. In case of anisotropic media permittivity must be treated as a tensor $\hat{\epsilon}$.

$$\hat{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix}. \quad (\text{B.1})$$

B.1 The wave equation with permittivity tensor

The intensities of electric and magnetic fields must obey Maxwell's equations. For this reason, we have to derive the wave equation. We start with equations

$$\mathbf{k} \times \mathbf{H}_0 + \omega \epsilon_0 \hat{\epsilon} \mathbf{E}_0 = 0, \quad \mathbf{k} \times \mathbf{E}_0 + \omega \mu_0 \hat{\mu} \mathbf{H}_0 = 0, \quad (\text{B.2})$$

where \mathbf{k} is the wavevector, \mathbf{E}_0 and \mathbf{H}_0 denote to the amplitudes of electric and magnetic field intensities respectively. ω is the angular frequency of electromagnetic wave. It should be mentioned that magnetic permeability tensor $\hat{\mu}$ can be neglected because optical or near-optical frequencies are too high for magnetic interactions. With use of identities

$$\mathbf{k} \times \mathbf{k} \times \mathbf{E}_0 = (\mathbf{k} \cdot \mathbf{E}_0) \mathbf{k} - (\mathbf{k} \cdot \mathbf{k}) \mathbf{E}_0, \quad \mu_0 = \frac{1}{\epsilon_0 c^2}, \quad k_0 = \frac{\omega}{c}, \quad (\text{B.3})$$

the wave equation becomes

$$(\mathbf{k} \cdot \mathbf{E}_0) \mathbf{k} - (\mathbf{k} \cdot \mathbf{k}) \mathbf{E}_0 + k_0^2 \hat{\epsilon} \mathbf{E}_0 = \bar{0}. \quad (\text{B.4})$$

We used $\bar{0}$ here to indicate that it is vector with zeros only. Obtained equation must be solved for each of N layers. Now, we should do one additional modification of the wave vector. Thanks to chose of the coordinate system we have

$$\mathbf{k} = \begin{pmatrix} 0 \\ k_y \\ k_z \end{pmatrix} = k_0 \begin{pmatrix} 0 \\ N_y \\ N_z \end{pmatrix} = k_0 \mathbf{N}, \quad (\text{B.5})$$

where $N_y = n_0 \cdot \sin \theta_0$ is identical in each layer due to the conservation of tangential component of the wave vector. $N_z = n \cdot \cos \theta$ is z -component of generalized refractive index. This quantity is generally different in each layer, later there will be added an index to note it. With this new notation the wave equation becomes

$$(\mathbf{N} \cdot \mathbf{E}_0) \mathbf{N} - (\mathbf{N} \cdot \mathbf{N}) \mathbf{E}_0 + \hat{\epsilon} \mathbf{E}_0 = \bar{0} \quad (\text{B.6})$$

$$\Downarrow$$

$$\begin{pmatrix} \epsilon_{xx} - N_y^2 - N_z^2 & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} - N_z^2 & \epsilon_{yz} + N_y N_z \\ \epsilon_{zx} & \epsilon_{zy} + N_y N_z & \epsilon_{zz} - N_y^2 \end{pmatrix} \begin{pmatrix} E_{0x} \\ E_{0y} \\ E_{0z} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \quad (\text{B.7})$$

In order to get non-trivial solution, the determinant of this matrix must be equal to zero. From that condition we would see that solution for N_z is given by equation

$$aN_z^4 + bN_z^3 + cN_z^2 + dN_z + e = 0 \quad (\text{B.8})$$

\Downarrow

$$\{N_{z1}, N_{z2}, N_{z3}, N_{z4}\}. \quad (\text{B.9})$$

It can be interpreted in the following way: there are four modes propagating in each layer. In a given coordinate system N_{z1} , N_{z3} are forward propagating and N_{z2} , N_{z4} are backward propagating modes. Sometimes, in case of higher optical symmetry of a given material, it turns out that $b = d = 0$. Then we obtain $N_{z1} = -N_{z2}$ and $N_{z3} = -N_{z4}$. We can say that N_{zj} are eigenvalues of matrix in equation B.7. It means that we can find its eigenvectors too. They are

$$\mathbf{E}_{j0} = A_j \mathbf{e}_j, \quad (\text{B.10})$$

where \mathbf{e}_j is eigen-polarization of j -th mode. From Maxwell equations we are able calculate amplitudes of magnetic field intensity of each mode in a given layer:

$$\mathbf{H}_{j0} = \frac{1}{\omega \mu_0} \mathbf{k} \times \mathbf{E}_{j0} = \sqrt{\frac{\epsilon_0}{\mu_0}} \mathbf{h}_j. \quad (\text{B.11})$$

In practice, this calculation must be performed in each of N layers. Next, we know that tangential components of electric and magnetic field intensity vectors must be equal at the boundaries. Let us assume boundary between $(n-1)$ -th and n -th layer. The boundary conditions can be summarized as

$$E_x^{(n-1)} = E_x^{(n)}, \quad E_y^{(n-1)} = E_y^{(n)}, \quad H_x^{(n-1)} = H_x^{(n)}, \quad H_y^{(n-1)} = H_y^{(n)}. \quad (\text{B.12})$$

Let us now take for example E_x and write it in terms of eigen-modes. It is

$$\sum_{j=1}^4 A_j^{(n-1)} e_{xj}^{(n-1)} = \sum_{j=1}^4 A_j^{(n)} e_{xj}^{(n)} \exp[ik_0 N_{zj}^{(n)} d_n]. \quad (\text{B.13})$$

B.2 Yeh's matrix formalism

When we write down all boundary conditions we obtain system of four equations which can be expressed using matrices as [3]

$$\mathbf{D}^{(n-1)} \mathbf{A}^{(n-1)} = \mathbf{D}^{(n)} \mathbf{P}^{(n)} \mathbf{A}^{(n)}, \quad (\text{B.14})$$

where $\mathbf{D}^{(n)}$ and $\mathbf{P}^{(n)}$ are called the dynamic and propagation matrix of n -th layer respectively. Let us express them exactly [24, 3]

$$\mathbf{D}^{(n)} = \begin{pmatrix} e_{x1}^{(n)} & e_{x2}^{(n)} & e_{x3}^{(n)} & e_{x4}^{(n)} \\ h_{y1}^{(n)} & h_{y2}^{(n)} & h_{y3}^{(n)} & h_{y4}^{(n)} \\ e_{y1}^{(n)} & e_{y2}^{(n)} & e_{y3}^{(n)} & e_{y4}^{(n)} \\ h_{x1}^{(n)} & h_{x2}^{(n)} & h_{x3}^{(n)} & h_{x4}^{(n)} \end{pmatrix}, \quad (\text{B.15})$$

$$\mathbf{P}^{(n)} = \begin{pmatrix} e^{ik_0 N_{z1}^{(n)} d_n} & 0 & 0 & 0 \\ 0 & e^{ik_0 N_{z2}^{(n)} d_n} & 0 & 0 \\ 0 & 0 & e^{ik_0 N_{z3}^{(n)} d_n} & 0 \\ 0 & 0 & 0 & e^{ik_0 N_{z4}^{(n)} d_n} \end{pmatrix}. \quad (\text{B.16})$$

If we wanted to obtain relation between $\mathbf{A}^{(n-1)}$ and $\mathbf{A}^{(n)}$, we would just multiply boundary condition relation by $[\mathbf{D}^{(n-1)}]^{-1}$ from left. Thus, we have

$$\mathbf{A}^{(n-1)} = [\mathbf{D}^{(n-1)}]^{-1} \mathbf{D}^{(n)} \mathbf{P}^{(n)} \mathbf{A}^{(n)}. \quad (\text{B.17})$$

This can be extended in order to describe entire system of N layers. It will be clear if we express $\mathbf{A}^{(n)}$ using matrices of $(n+1)$ -th layer:

$$\mathbf{A}^{(n)} = [\mathbf{D}^{(n)}]^{-1} \mathbf{D}^{(n+1)} \mathbf{P}^{(n+1)} \mathbf{A}^{(n+1)} \quad (\text{B.18})$$

\Downarrow

$$\mathbf{A}^{(n-1)} = [\mathbf{D}^{(n-1)}]^{-1} \mathbf{D}^{(n)} \mathbf{P}^{(n)} [\mathbf{D}^{(n)}]^{-1} \mathbf{D}^{(n+1)} \mathbf{P}^{(n+1)} \mathbf{A}^{(n+1)}. \quad (\text{B.19})$$

Now, the recursion is obvious and we can write the relation between $\mathbf{A}^{(0)}$ and $\mathbf{A}^{(N+1)}$. It is

$$\mathbf{A}^{(0)} = [\mathbf{D}^{(0)}]^{-1} \mathbf{D}^{(1)} \mathbf{P}^{(1)} \dots [\mathbf{D}^{(N)}]^{-1} \mathbf{D}^{(N+1)} \mathbf{A}^{(N+1)}, \quad (\text{B.20})$$

where $[\mathbf{D}^{(0)}]^{-1} \mathbf{D}^{(1)} \mathbf{P}^{(1)} \dots [\mathbf{D}^{(N)}]^{-1} \mathbf{D}^{(N+1)} = \mathbf{M}$ is called the total matrix of the system. From this matrix we are able to calculate the amplitude reflection and transmission coefficients or for example electric field distribution in entire multilayer [24, 3].

In case of isotropic layers the calculations are lot simpler. We do not have to describe optical properties using tensor. Permittivity is just scalar quantity. After performing practically identical calculations we would find out that dynamic matrix of n -th layer is

$$\mathbf{D}^{(n)} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ n^{(n)} \cos \theta^{(n)} & -n^{(n)} \cos \theta^{(n)} & 0 & 0 \\ 0 & 0 & \cos \theta^{(n)} & \cos \theta^{(n)} \\ 0 & 0 & -n^{(n)} & n^{(n)} \end{pmatrix}. \quad (\text{B.21})$$

It means that we can separately describe s- and p- polarizations. We can see that dynamic matrix of isotropic layer contains four blocks of dimensions 2×2 . Those with non-zero elements are in fact dynamic matrices of n -th layer for s- and p-polarizations respectively [3].

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